The Impact of Molecular Chlorine Emissions on Ozone Formation in Southeast Texas

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Summary

The objectives of this project were to determine the effect of chlorine on the kinetics of ozone formation in a mixture representing the atmosphere of a coastal urban center and to identify hydrocarbon maker species that can assist in characterizing the extent of chlorine reactions in the gas phase. A smog chamber was designed and constructed in order to conduct these experiments and series of chamber experiments were run. Injection of chlorine into a simulated urban air mass resulted in a dramatic increase in ozone production. While no chlorinated marker species could be found, it was determined that the relative reactivities of VOCs can be used to determine if chlorine chemistry occurs to a significant extent.

Using the results of the smog chamber experiments, the potential impact of chlorine chemistry on ozone formation in Southeast Texas was assessed for an episode that occurred on August 19, 1993. This date was chosen for analysis because ozone formation, at selected monitoring sites, could not be explained using existing chemical mechanisms. Backtrajectories calculated by the TNRCC revealed that the air parcel arriving at the site with unusually high ozone concentrations had passed over a chlorine source and had initially contained high concentrations of alkanes, which reacted by the time the air parcel arrived at the downwind monitoring site. These observations are consistent with the chemistry observed in the smog chamber experiments, suggesting that molecular chlorine chemistry may play a significant role in some ozone episodes.

Finally, in a supplement to this report a simplified set of chemical reactions describing the role of chlorine in ozone formation is proposed. This mechanism is designed to be used in conjunction with the CBIV mechanism commonly used in regional photochemical models.

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CHAPTER 1: INTRODUCTION

Oxidation reactions control the fate of most volatile organic compounds (VOCs) and nitrogen oxides (NO_x) in the troposphere. These reactions are dominated by photochemically produced hydroxyl radicals (OH^*) during the day, and nitrate radicals (NO_3^*) at night and in polluted areas. However, recent studies have indicated that halogen species, such as chlorine, may contribute to, or even locally dominate, the oxidative chemistry in the lower troposphere.[1] The photolysis of molecular chlorine provides a source of radicals that dramatically increases oxidation and ozone formation processes.

Chlorine can be generated in the troposphere through several mechanisms. It has been well documented that in the marine boundary layer gas-phase atomic chlorine can be generated by reactions of sea-salts. One of the reactions that generates chlorine atom precursors is that of sodium chloride with NO_x. Recent studies also suggest that molecular chlorine can be formed from the reactions of ozone (O_3) with sea-salt particles.[1,2] Molecular chlorine (Cl_2) has recently been directly measured in a coastal area at concentrations up to 150 ppt, and it is estimated that a yet unrecognized source must exist that produces up to 330 ppt of Cl_2 daily.[1, 2] Large amounts of chlorine and chlorine atom precursors are also released from certain anthropogenic sources.[3, 4] Some of these include petroleum refineries, chlor-alkali facilities, chlorinated chemical manufacturing operations, and other industrial facilities.

The cycling of atomic chlorine can provide either a source or sink for ozone. In a low NO_x environment, chlorine atoms can destroy ozone through direct reaction. Ozone loss occurs through the following reactions[5]:

$$Cl^* + O_3 \rightarrow ClO^* + O_2 \quad (1.1)$$
$$ClO^* + HO_2^* \rightarrow HOCl + O_2 \quad (1.2)$$
$$HOCl + h\nu \rightarrow OH^* + Cl^* \quad (1.3)$$

The overall net reaction is:

$$O_3 + HO_2^* \rightarrow OH^* + 2O_2 \quad (1.4)$$

In contrast, when there are sufficient hydrocarbons and oxides of nitrogen, the chlorine radicals can react with the VOCs to form ozone. Briefly, the ozone generation cycle due to chlorine and hydroxyl reactions is as follows[4,6]:

$$RH + OH^*(\text{or } Cl^*) \rightarrow R^* + H_2O \text{ (or HCl)} \quad (1.5)$$
$$R^* + O_2 \rightarrow ROO^* \quad (1.6)$$
$$ROO^* + NO \rightarrow NO_2 + RO^* \quad (1.7)$$
$$RO^* + O_2 \rightarrow HOO^* + \text{carbonyl} \quad (1.8)$$
$$HOO^* + NO \rightarrow NO_2 + OH^* \quad (1.9)$$
$$NO_2 + h\nu \rightarrow NO + O^*(^3P) \quad (1.10)$$
$$O^*(^3P) + O_2 + M \rightarrow O_3 \quad (1.11)$$
$$O_3 + NO \rightarrow NO_2 + O_2 \quad (1.12)$$

In addition to chlorine (Cl^*) being a source of radicals, the rate of reaction of Cl^* with organics is significantly different than that of the hydroxyl radicals (OH^*). This is important since the rate constants determine how fast the organic can convert NO to NO_2 and consequently how fast ozone is formed.

The objective of this project is to examine the role of molecular and atomic chlorine in affecting ozone formation chemistry under urban conditions. Specifically, there are three major objectives.

1. determine the effect of molecular chlorine on the kinetics of ozone formation in a mixture representing the atmosphere of a coastal urban center
2. identify hydrocarbon marker species that can assist in characterizing the extent of chlorine reactions
3. examine ambient air quality data from Southeast Texas for evidence of chlorine chemistry

An outdoor smog chamber was designed and constructed in order to gain a better understanding of reactions that generate photochemical smog. Four separate smog chamber experiments were conducted in this study. In each run approximately 85 ppb_v of NO_x and 110 ppb_v (1100 ppb_C) of a hydrocarbon mixture were added to simulate an urban air parcel. Next, chlorine was injected in to the chamber in three of the experiments in amounts ranging from 12 ppb_v, to 40 ppb_v. The ozone and NO_x concentrations were continuously monitored during a 3 to 5 hour sampling time. Additionally, a hydrocarbon sample taken before and after each experiment was analyzed to assess the relative reactivities of the hydrocarbons.

The experiments resulted in two main findings. First, the injection of chlorine into the simulated urban air resulted in a dramatic increase in ozone production. The control run, in which no chlorine was injected, only produced 40 ppb_v of ozone. However, the experiments with chlorine injection yielded ozone concentration ranging from 83 to 262 ppb_v. Second, while no chlorinated hydrocarbon reaction product could be found, the relative reactivities of the VOCs used in the experiments with chlorine injection were significantly different than the relative reactivities for experiments with no chlorine injection. The alkanes and substituted alkanes, which typically do not react rapidly with hydroxyl radicals, reacted rapidly in the experiments with chlorine injection. In contrast, the concentration of olefins and aromatics were consistent between the experiments with injected chlorine and the control experiment. Thus, decreased concentrations of alkanes and substituted alkanes in ambient air samples could serve as an indicator that chlorine chemistry is occurring, and ambient air quality data from Southeast Texas were examined for this evidence of chlorine chemistry.

CHAPTER 2: THEORETICAL BACKGROUND

2.1 Atmospheric Chemistry of the Troposphere

The gas-phase chemistry of the troposphere involves the photoxidation of volatile organic compounds (VOCs) in the presence of oxides of nitrogen (NO_x). Ozone can be considered one of the principal products of this chemistry. The amount of ozone produced is strongly dependent on the ultraviolet sunlight intensity, the concentration of VOCs and NO_x in the lower atmosphere, temperature, humidity, and cloud cover. Ozone can irritate the eyes and respiratory passages causing breathing difficulties and may increase susceptibility to infection. It is a highly reactive chemical, capable of attacking surfaces, fabrics, and rubber materials. Ozone is also toxic to some crops, vegetation, and trees. The amount of ozone produced is a non-linear function of reactive organic gases and oxides of nitrogen.[7, 8]

The atmospheric chemistry involved in ozone formation is complex, involving many constituents and side reactions. However, cycles of free radical reactions drive the chemistry, and include reactions involving reactive organic gases, hydroxyl radicals, oxides of nitrogen, and ozone. The following mechanisms briefly summarize this complex chemistry. A central element involves the chemistry of NO_x.[7, 8]

$$NO_2 + h\nu \rightarrow NO + O^*(^3P) \qquad (2.1.1)$$
$$O^*(^3P) + O_2 + M \rightarrow O_3 \qquad (2.1.2)$$
$$O_3 + NO \rightarrow NO_2 + O_2 \qquad (2.1.3)$$

These reactions occur rapidly and in the absence of VOCs yield a steady state ozone concentration. Reaction 2.1.3 acts as an ozone sink. O^* represents a highly reactive oxygen atom that has an unpaired electron, and M represents any third body which is usually N_2.

When volatile organic compounds are included in the chemistry, higher ozone concentrations result because of both an increase in O_3 sources and a reduction in the O_3 sinks. The following equations show a simplified version of the VOC chemistry where RH represents any volatile organic compound that reacts with a hydroxyl radical (OH^*) to form alkyl radicals (R^*).

$$RH + OH^* \rightarrow R^* + H_2O \qquad (2.1.4)$$
$$R^* + O_2 \rightarrow ROO^* \qquad (2.1.5)$$
$$ROO^* + NO \rightarrow NO_2 + RO^* \qquad (2.1.6)$$

One particular set of reactions to note is the formation and reduction of the peroxyradical, ROO^*. These steps allow ozone to accumulate by reducing the ozone sink (NO) and increasing ozone sources (NO_2).

The presence of hydroxyl radicals is essential for O_3 formation; it's key role being the conversion of volatile organic compounds to peroxyradicals. The formation of hydroxyl radicals involves the photolysis of carbonyls and the following two reactions.[7, 8]

$$O^*(^1D) + H_2O \rightarrow 2OH^* \qquad (2.1.7)$$

$$HOO^* + NO \rightarrow NO_2 + OH^* \qquad (2.1.8)$$

Also OH^* and NO_2 may react to form nitric acid,

$$OH^* + NO_2 \rightarrow HNO_3 \qquad (2.1.9)$$

Another way hydroxyl radicals are formed is by the photodissociation of ozone, which produces atomic oxygen, which then reacts with water vapor.[7]

$$O_3 + h\nu \rightarrow O^* + O_2 \qquad (2.1.10)$$
$$O^*(^1D) + H_2O \rightarrow 2OH^* \qquad (2.1.11)$$

2.2 Chlorine Chemistry and Interactions with Ozone Chemistry

Since chemical sink processes of tropospheric gases are generally assumed to be dominated by the reactions of OH and O_3, the potential contribution of atomic and molecular chlorine has been neglected. The role of chlorine is to provide a source of radicals that speed up the ozone formation process and enhance the ozone forming potential of the ozone precursors in ambient air.[4] Chlorine chemistry is particularly important since chlorine atoms compete with the hydroxyl radical (OH^*) in photochemical reactions. This especially effects the atmospheric removal rates of volatile organic compounds.

Chlorine, Cl_2, is photodissociated by visible and ultraviolet light:

$$Cl_2 + h\nu \rightarrow Cl^* + Cl^* \qquad (2.2.1).$$

Hov[3] calculated the dissociation rate constants for this reaction. The maximum calculated value for $k_{2.2.1}$ was 1.6×10^{-3} s^{-1} based on the standard absorption cross sections published by NASA.[3] The characteristic time for Cl_2 photodissociation varies from about 10 minutes at noon in midsummer, to about 20 minutes at noon in February. This implies that Cl_2 is photodissociated rapidly during all seasons and is an immediate source of chlorine atoms as soon as it is released.[3]

Once atomic chlorine is formed in the troposphere it can react either with ozone or organics:

$$Cl^* + O_3 \rightarrow ClO^* + O_2 \qquad (2.2.2)$$
$$RH + Cl^* \rightarrow R^* + HCl \qquad (2.2.3)$$

Which reaction is more significant can be determined by the rate of Cl^* removal, d[Cl]/dt. Finlayson-Pitts calculated d[Cl]/dt for both equations by assuming an O_3 concentration of 35 ppb_v and an organic concentration of 75 ppb_v which are typical marine troposphere levels and rate constants of $k_{2.2.2}=1.1 \times 10^{-11}$ and $k_{2.2.3}=1 \times 10^{-10}$ cm^3 mol^{-1} s^{-1}. This resulted in a d[Cl]/dt for reaction 2.2.2 of approximately 10 s^{-1} and for reaction 2.2.3 approximately 200 s^{-1}.[9] Thus, organics, rather than ozone, are the preferred removal route by chlorine atoms in the marine troposphere. Since similar ratios of hydrocarbon to ozone are observed in urban atmospheres (1000 ppb_C hydrocarbons to 100 ppb_v ozone), hydrocarbons should also dominate atomic chlorine reactions in urban atmospheres.

The cycling of atomic chlorine could provide either a source or sink for ozone depending on the NO_x concentrations. Chlorine chemistry modifies the photochemical smog mechanism in several ways. First, an ozone sink results from the following reactions[5]:

$$Cl^* + O_3 \rightarrow ClO^* + O_2 \qquad (2.2.4)$$
$$ClO^* + HO_2^* \rightarrow HOCl + O_2 \qquad (2.2.5)$$
$$HOCl + h\nu \rightarrow OH^* + Cl^* \qquad (2.2.6).$$

The net overall reaction is:

$$Cl^* + O_3 + HO_2^* \rightarrow Cl^* + 2O_2 + OH^* \qquad (2.2.7).$$

It is interesting to note here that reaction 2.2.7 is autocatalytic with respect to atomic chlorine.

This sink for ozone can be compensated for by the production of hydroxyl radicals from the oxidation of volatile organic compounds. This leads to increased ozone production in the presence of sufficient NO_x.[2,4,5] Briefly, the ozone generation cycle with chlorine and hydroxyl interactions is as follows[4,6]:

$$RH + Cl^* (\text{ or } OH^*) \rightarrow R^* + HCl (\text{ or } H_2O) \qquad (2.2.8)$$
$$R^* + O_2 \rightarrow ROO^* \qquad (2.2.9)$$
$$ROO^* + NO \rightarrow NO_2 + RO^* \qquad (2.2.10)$$
$$RO^* + O_2 \rightarrow HOO^* + \text{carbonyl} \qquad (2.2.11)$$
$$HOO^* + NO \rightarrow NO_2 + OH^* \qquad (2.2.12)$$

The important reactions here are the ones that oxidize NO to NO_2 since they control the steady state concentration of O_3.

$$NO_2 + h\nu \rightarrow NO + O^* \qquad (2.2.13)$$
$$O^* + O_2 + M \rightarrow O_3 \qquad (2.2.14)$$
$$O_3 + NO \rightarrow NO_2 + O_2 \qquad (2.2.15)$$

In this mechanism, ozone builds up whenever NO is converted to NO_2 without the loss of O_3. Thus, chlorine atoms may initiate organic oxidation in a mechanism similar to that of hydroxyl radicals, which accelerate the formation of ozone.[6] However, if there is not a sufficient source of NO_x then atomic chlorine can actually act as an ozone sink.

This is only a brief discussion of the interactions of chlorine to produce photochemical smog. A more detailed mechanism, complete with rate constants, has been compiled by Whitten, Johnson, and Killus.[4]

2.3 Atmospheric Chlorine

Molecular chlorine is emitted to the troposphere from various sources. Currently, there is no method to allow the direct measurement for chlorine atoms at ultra-trace levels and sources differ widely on estimated tropospheric levels.[10] However, recently strong evidence has been assembled in support of significant levels of halogen atoms and the oxidation of organic species

by halogens.[10,11] Chlorine atom concentrations are determined indirectly by observing the changes in the patterns of non-methane hydrocarbons over the ocean. A study using this technique conducted by Ramacher et al.[11] reported integrated chlorine atom concentrations of approximately 5±14 x 10^8 s/cm^3 at background ozone concentrations of 30 ppb_v in the marine troposphere. Keene and Graedel report that the typical background abundance of reactive chlorine in the lower troposphere is about 1.5 ppb_v.[12] This is composed of about nine species: CH_3Cl, CH_3CCl_3, HCl, $CHClF_2$, Cl_2, CCl_2CCl_2, CH_2Cl_2, $COCl_2$, and $CHCl_3$. The total tropospheric reactive chlorine burden is approximately 8.3 Tg Cl, and is expected to increase in the next several decades especially near urban areas in rapidly developing countries.[12]

One of the sources of chlorine is anthropogenic sources. In the Salt Lake City region, one facility alone emits 44,300 tons/year of Cl_2 and 440 tons/year of HCl.[4] Hov also studied an industrial region in southern Telemark, Norway which had several large industrial sources of chlorine that significantly changed the photoxidative chemistry in the region.[3] The greater Houston, Texas region also contains many large anthropogenic sources of chlorine. The largest such emitter released 16 million pounds in 1993 through a continuous stack release, as reported through the Toxic Release Inventory. Figure 2.1 below displays the location of this industrial facility (indicated with a triangle). The second largest emitter in 1993 released 6.14 million pounds of chlorine due to fugitive emissions and the third largest released approximately 3 million pounds of chlorine through a stack release.[13] These facilities are also labeled with a triangle.

Figure 2.1 Map of Three Largest Chlorine Sources in Houston in 1993

Molecular chlorine is also photolytically produced from reactions with sodium chloride, a major component of sea-salt particles, and ozone when the sea-salt particles are above their deliquescence point.[2,9] Chlorine is also released in the form of organohalogen compounds from many natural sources such as marine algae, phytoplankton, fungi, biomass burning, and volcanic eruptions. Global emissions of chloromethane alone from marine and terrestrial biomass are five million tons per year. [14] Other unusual events such as the burning of the oil fields in Kuwait have also generated significantly high levels of chlorine.[2,9]

2.4 Organic Reactivity

It is often difficult to express the reactivity of an organic using only one measure that can encompass all the aspects of its complex atmospheric chemistry. Reactivity is often summarized by discussing it in terms of reaction rate measures, which include the rate of NO_2 formation, the rate of organic consumption, and the rate of ozone formation, and in terms of product yield measures, which include maximum concentration of ozone achieved, total ozone dosage over a fixed time of irradiation, and maximum concentration of peroxyacetal nitrate (PAN) achieved.[7] One of the factors that must be considered in defining the reactivity of organics is their respective rate of reaction, either with OH^* or Cl^*, since this determines how fast the organic can convert NO to NO_2 and consequently how fast ozone is formed. Also, the radical concentrations of either OH^* or Cl^* in the mixture, will significantly affect the level of photoxidation.[7]

To further demonstrate this concept, a set of representative hydrocarbons have been chosen to show how the rate constant can affect the relative importance of Cl^* or OH^* pathways. The sample set includes an alkane, a substituted alkane, an olefin, a substituted olefin, an aromatic, and a substituted aromatic. The rate constants shown in Table 2.1 correspond to the following equations:

$$OH^* + HC \rightarrow \text{products} \qquad (2.4.1)$$
$$Cl^* + HC \rightarrow \text{products} \qquad (2.4.2)$$

Table 2.1 Rate Constants for a Representative Set of Hydrocarbons

Hydrocarbon (HC)	k_{OH*} ($k_{2.4.1}$)	k_{Cl*} ($k_{2.4.2}$)	k_{Cl}/k_{OH}
Hexane	545×10^{-14} [a]	$34{,}000 \times 10^{-14}$ [a]	62
2,4 Dimethyl Pentane	500×10^{-14} [a]	$29{,}000 \times 10^{-14}$ [a]	58
1-Propene	$2{,}630 \times 10^{-14}$ [a]	$28{,}000 \times 10^{-14}$ [a]	11
2-Methyl 1-3 Butadiene	$10{,}100 \times 10^{-14}$ [a]	$48{,}000 \times 10^{-14}$ [a]	5
Benzene	91.1×10^{-14} [b]	0.9×10^{-14} [c]	0.01
Toluene	758×10^{-14} [b]	$5{,}890 \times 10^{-14}$ [d]	8

All Rate constants, k, have units of cm^3 molecule $^{-1}$ s^{-1} and are at 1 atm.
[a] Rate constants are at 298K (Atkinson, 1997).[15]
[b] Rate constants are at 250 K (Atkinson, 1986).[16]
[c] Rate constants are at 298K (Ariya, 1996).[11]
[d] Rate constants are at 298 (Atkinson and Ashmann, 1985).[17]

As seen in table 2.1, chlorine atoms react rapidly in comparison to hydroxyl radicals with hydrocarbons. The ratio of rate constants for the reactions of alkanes (paraffins) chlorine radical relative to reactions with the hydroxyl radical, k_{Cl*}/k_{OH*}, is approximately 100 while the corresponding ratio with alkenes (olefins) is approximately 10. Thus chlorine atom reaction with alkenes are generally of less importance as a tropospheric loss process than alkanes.[15] Benzene is more reactive with hydroxyl radicals than with chlorine radicals, while toluene appears to behave similar to the alkenes, slightly favoring the chlorine reaction.

2.5 Outdoor Smog Chambers

A smog chamber is a batch reactor that is used to gain an understanding of reactions that generate photochemical smog, and to develop strategies of smog abatement. There are two types of smog chambers, indoor and outdoor. Outdoor chambers use natural conditions of light, temperature, and humidity to simulate conditions in urban atmospheres.[19] Indoor chambers must use artificial light sources to simulate natural light intensity. They are not always characteristic of true atmospheric chemistry since they typically cannot simulate natural conditions, such as diurnal light intensity, that are crucial to oxidant control strategies.[19] However, in some circumstances, for example, in determining complex mechanisms in smog reactions, indoor chamber experiments are more useful because they can determine precise data under controlled conditions.[20]

Many chamber bags are constructed out of a fluorinated ethylene-propylene copolymer (FEP Teflon) that is heat sealed around the edges to form a “pillow- like” structure. FEP Teflon is an excellent material for a smog bag since the surface has a very high transmission for the entire solar spectrum and only exhibits a few absorption bands in the IR, which reduces the “greenhouse effect”.[19,21] In fact, in studies conducted by Kelly 0.05 mm, FEP teflon film transmitted over 95% of the full solar spectrum at wavelengths greater than 300nm.[22] However, this thin Teflon film is usually very fragile. Teflon fittings are also typically attached to the bag for sampling, filling, and cleaning the bag.

There are many factors that could possibly affect the results from smog chamber experiments such as the effects of spectral distribution, wall materials, and chamber cleanup or preparation procedures. If FEP Teflon is used in an outdoor chamber, then spectral distribution should not be a significant error. However, the effects of wall conditioning and contamination are potentially very important sources of error for Teflon chambers.[21,22] Lonneman[5c] et al reported that depending on the batch of bags and the manufacturer, some new FEP Teflon film released large amounts of volatile residues from the film manufacturing process.[21] Other researchers have reported that used Teflon bags exhibit greater reactivity and increased ozone production than new bags due to the release of products from the Teflon left from previous experiments. Additionally, teflon is permeable to a wide variety of compounds.[22] Daubendiek and Calvert report that ozone and Teflon can react with each other and introduce the possibility of gas-phase products.[23] However, Kelly observed after performing a series of experiments that there was no significant contamination in experiments that used at least moderate levels of oxides of nitrogen.[22] This was because at low NO_x environments ozone formation was independent of added VOCs. [22] However, Kelly did state that different batches of Teflon film may contain greater amounts of initial contaminants than they observed. It is recommended that to avoid these possible errors, new bags be conditioned for photolysis experiments by filing with clean dry (zero) air or zero air plus ozone and irradiating for 1 day. [19,21,22,23]

CHAPTER 3: METHODOLOGY

3.1 Construction of the Smog Chamber

The smog chamber bags that were designed for the purposes of this work were constructed out of 5mil thick, clear, fluorinated ethylene-propylene copolymer (FEP Teflon, type A). Norton Chemical Company performed the delicate fabrication by heat sealing two sheets of the FEP Teflon around the edges to form a "pillow- like" structure. Each bag was approximately 15 feet long and 5 feet wide. When fully inflated, a bag was about 4 feet tall with an internal volume of approximately 2400 liters. Swagelok™ fittings also made of teflon were attached to the bag for sampling, filling, and cleaning the bag. Additional teflon material on each end of the bag contained a metal ring infused in the teflon in order to suspend the bag. A large frame was constructed from metal pieces called Unistrut™. Each bag was then tied in to the frame with nylon rope so that it was entirely free standing with no contact with any material. Figures 3.1 and 3.2 are photographs of the smog chamber when it is half-filled. The frame was built to reside outdoors at the J.J. Pickle Research Campus at 10100 Burnet Road in Austin, Texas.

The effects of wall conditioning and contamination are potentially very important sources of error for Teflon chambers. In order to limit contamination each bag was initially filled with zero air early in the morning and allowed to bake for several hours in the sun. Then one port was opened with the zero air still running and the bag was allowed to flush for about an hour. Next, the bag was pumped out so that there was no gas remaining and refilled with fresh zero air. If the bag had never been used before this procedure was lengthened and performed the day before instead of just the morning of the experiment.

Prior to each smog chamber experiment, the bag was filled with approximately 2300 to 2500 liters of zero air. Next it was covered with an opaque black tarp made out of Visqueen™ so that no sunlight was introduced until the experiment was ready to begin. Ten liters of a NO_x mixture and five liters of a hydrocarbon mixture were used in each experiment so that the only variable was the chlorine concentration. The NO_x mixture was from a Praxair cylinder, which contained 20.2 ppm_v NO_x (which was 20.1 ppm_v NO) in nitrogen. The hydrocarbon mixture was the Matheson "Enviro-MAT™ Ozone Precursor Mixture. It contained 56 separate VOCs all at a 1 ppm_v concentration. Table 3.1 lists all of the VOCs in the mixture.

Figure 3.1 Horizontal View of Smog Chamber

Figure 3.2 Vertical View of Smog Chamber

Table 3.1 List of Components for Enviro-MAT™ Ozone Precursor

ethane	2-methylhexane	3-methyl-1-butene
propane	2-methylheptane	2-methyl-1-pentene
isobutane	3-methylheptane	4-methyl-1-pentene
n-butane	cyclopentane	cyclopentene
isopentane	cyclohexane	isoprene
n-pentane	methylcyclopentane	alpha-pinene
n-hexane	methylcyclohexane	beta-pinene
n-heptane	acetylene	benzene
n-octane	ethylene	toluene
n-nonane	propylene	m-xylene
2,3-dimethylbutane	1-butene	o-xylene
2,4-dimethylbutane	cis-2-butene	p-xylene
2-methylpentane	trans-2-butene	stryrene
3-methylpentane	1-pentene	ethylbenzene
2,3-dimethylpentane	cis-2-pentene	1,2,4-trimethylbenzene
2,4-dimethylpentane	trans-2-pentene	1,3,5-trimethylbenzene
1,3,4-trimethylpentane	cis-2-hexene	n-propylbenzene
2,2,4-trimethylpentane	trans-2-hexene	isopropylbenzene
3-methylhexane	2-methyl-2-butene	

This made the concentration for NO_x in each experiment approximately 85 ppb_v and the concentration of each individual VOC approximately 2 ppb_v, corresponding to a total VOC concentration that averaged approximately 1200 ppb_c over all of the experiments. The NO_x and VOCs were added to smog chamber using Nalgene tubing (purchased from Fisher Scientific), connected to 2 mil Tedlar sample bags (from SKC Sample Collection Media). Each Tedlar sample bag was 5 liters in volume and was filled with either NO_x or VOCs and then emptied in to the chamber through the tubing. All of the tubing connections in the entire experiment were Swagelok parts made from Teflon.

The NO_x and VOC mixtures were added to the smog chamber while it was covered by the black tarp. Next, depending on the individual run, chlorine gas (1000 ppm_v Cl_2 in nitrogen) was added using a syringe and a septum attached to the smog chamber. Runs 1 through 3 used 30 cc (12 ppb_v), 100 cc (40 ppb_v), and 42 cc (16.5 ppb_v) of Cl_2 gas respectively. Run 4 was the control and did not have any chlorine injection. After Cl_2 injection the covered bag was then allowed to sit for approximately an hour so that it would be well-mixed. When each run finally began the black tarp was taken off and ozone and NO_x were measured continuously for about 3-5 hours. The NO_x and ozone analyzers remained in the laboratory and were connected through a small sampling port in the wall to the smog chamber by Nalgene tubing and Swagelok connections.

3.2 Sampling Methods

Four types of measurements were made during each smog chamber run: hydrocarbons, ozone, nitrogen oxide, and total oxides of nitrogen. Nitrogen dioxide was calculated by subtracting the NO from the total NO_x. The ozone and the oxides of nitrogen were sampled continuously throughout the experiment and the concentrations calculated using five minute time averages. The hydrocarbons were sampled once before each experiment was run and once after the experiment was completed. Table 3.2 presents a summary of the technologies that were used to make the measurements. Table 3.3 lists the quantitative objectives for data quality.

Table 3.2 Data Measurement Methods

Compound	*Method*	*Frequency*
Ozone	UV Photometry	Continuous
Nitrogen Oxide	Chemiluminescence	Continuous
Total NO_x	Chemiluminescence	Continuous
Hydrocarbons	GC/FID and GC/MS	Episodic

Table 3.3 Data Quality Objectives

Measurement	Method detection Limit
NO and NO_x	1.0 ppb_v
Hydrocarbons	2.5 ppbc (1)

(1) Hydrocarbons with 9 or more carbons per molecule may not meet this criterion.

3.2.1 OZONE AND OXIDES OF NITROGEN SAMPLING

Ozone was measured by ultraviolet absorption using a Dasibi Model 1008AH ozone analyzer. The analyzer was calibrated to operate in the range of 0 to 400 ppb_v with a sensitivity of 1 ppb_v. Every connection to the ozone photometric analyzer that contacted the sample was constructed of inert materials such as teflon or glass. A 5.0 μm teflon filter was placed in the air sampling line near the instrument inlet. The ozone monitor draws approximately 1.5 liters per minute of gas through the sampling line.

Oxides of nitrogen were measured using O_3 chemiluminescence using a Monitor Laboratories Model 9841 analyzer. The NO_x analyzer was calibrated to operate in the range of 0 to 470 ppb_v with a sensitivity of 1 ppb_v. All of the connections to the instrument that contacted the sample from the smog chamber were constructed of teflon, glass, or other inert materials. A 5.0 μm teflon filter was placed in the air sampling line near the instrument inlet. The NO_x analyzer draws approximately 1 liter per minute through the sampling line.

Calibrations of the NO_x and ozone analyzers were performed before the equipment was used in the fall and then again in the spring. The same NO_x and ozone analyzers were used throughout all of the experiments. The calibration of the equipment required the analysis of four standard concentrations, not including zero, without adjustment of the instrument. All of the gas standards used in the calibrations were from a source that was a known and documented concentration. Nitrogen oxide and nitrogen dioxide measurements were calibrated using a NO cylinder that was 20.1 ppm_v of NO in nitrogen from the Praxair Company. NO and NO_x

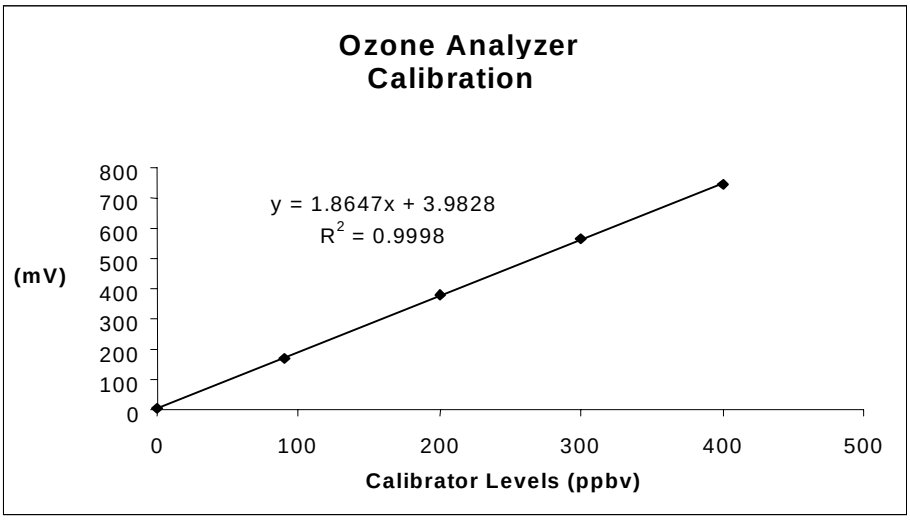


Figure 3.3 Typical calibration curve for the ozone analyzer

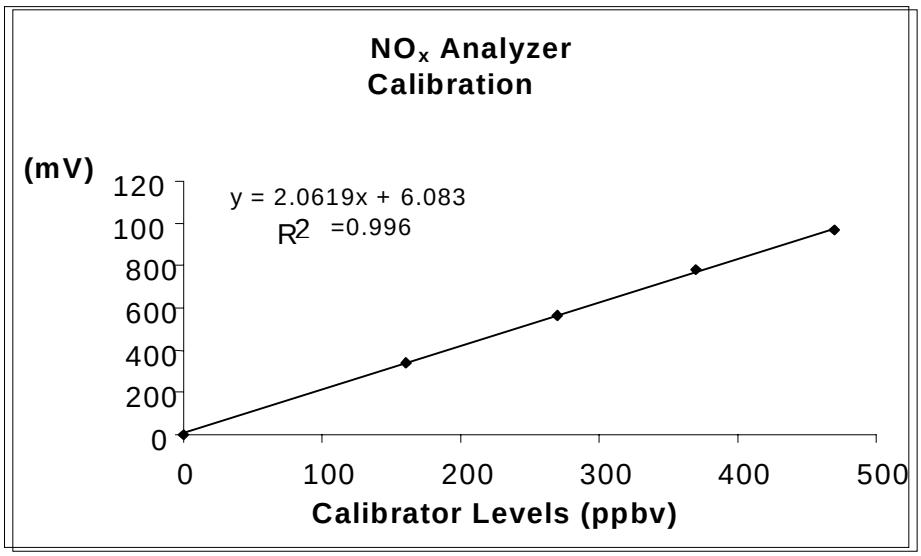


Figure 3.4 Typical calibration curve for the NO_x analyzer

calibrations were performed directly, while the NO_2 concentrations were determined by subtracting the NO from the total NO_x. The ozone used to calibrate the ozone analyzer was from the Dasibi Model 5008 programmable multi-gas calibrator. A minimum of five data points that spanned the working range of the analyzer were used to conduct the calibrations. Typical calibration curves are shown below in Figures 3.3 and 3.4.

3.2.2 SPECIATED NON-METHANE HYDROCARBONS

The hydrocarbon samples that were collected from the smog chamber experiments were collected using a volatile organic compound (VOC) assembly. The samples were collected using 6 liter Summa® passivated stainless steel canisters that were purchased from Meriter.

Sampling

Two hydrocarbon samples were taken during each experiment. The first one was taken after the mixture had been in the chamber for about an hour (to ensure a well-mixed sample) but before the chamber was exposed to ambient sunlight. The second sample was taken immediately after the experiment was completed. Each time the canister was attached to the bag using a 3 foot section of Teflon tubing and Swagelok™ fittings. The canister was then opened slowly by turning the valve, and allowed to fill entirely taking about 1 minute. After sampling, the canisters were taken to the laboratory for analysis. The VOC analysis assembly consisted of several sections: the doubler, the cryofocuser, the GC/FID, and the canister cleaner.

Doubler

First the canisters were sent to the doubler, which was designed and built by personnel at the Texas Natural Resource Conservation Commission (TNRCC). The doubler precisely doubles the canister pressure, so that the internal pressure is increased to above atmospheric pressure. The gauge pressure in the canisters after doubling is approximately 14.7 psig. A mass flow controller in the doubler was used to control the nitrogen that is used to double the volume in each canister. A pressure transducer in the doubler registered the precise pressure in the canister before and after dilution. A data logger controlled the total volume of nitrogen drawn in to the canister.

Cryofocusing and Data Collection

Next, the canisters were attached to the chemical analysis system. The system consisted of a cryofocuser, a gas chromatograph, and data acquisition system. An Entech 7000 preconcentrator combined 400 milliliters of the canister sample and 400 milliliters of an internal standard at 20 ppb_v per standard. The internal standard, which contained known amounts of organic gases, was added to assist in identifying unknown components in the smog chamber samples. The mixture was then cooled to -185°C, and the overhead gases were drawn off before the sample was reheated. The preconcentrator repeated this process three times so that the mixture volume was decreased to an order of a microliter, and the VOC concentration was increased many orders of magnitude. This is necessary so the detection system can identify and quantify the volatile organic compounds is the sample.

The chemical analysis system used was a Hewlett Packard 5890A gas chromatograph (GC) equipped with a flame ionization detector (FID) and a Hewlett Packard 6890 GC with a Hewlett Packard 5972 mass selective detector (MSD). The GC was fitted with a Hewlett Packard HP-1 column containing a 100% dimethylpolysiloxane coating, which enabled the retention of non-polar hydrocarbon species. The mixture then left the cryofocuser and was desorbed on the GC column. Next, a temperature ramping program was performed by the GC oven as shown in Table 3.4.

Table 3.4 Temperature Program for GC/FID Analysis System

Initial temperature (°C)	final temperature (°C)	temperature ramp (°C/min)	holding time at final temperature (min)
-10	-10	0	5
-10	0	5	0
0	120	10	2
120	160	4	6

For each gas sample sent to the GC, a chromatogram was generated using the EZ-Chrom V4.0 software. Estimates of the VOC concentrations were generated by determining the area of each peak and converting it to a concentration by using the appropriate calibration curve. Calibration curves were produced by using standard gas mixtures acquired from Wilson Oxygen and the Texas Natural Resource Conservation Commission (TNRCC). The internal standard contained 20 ppb_v of each of the following: 1,2-dichlorotetrafluoroethane, trifluoromethyl benzene, and 1,3-bromofluorobenzene. These three components appeared at early, mid and late points (respectively) in the chromatograms to assist in optimum identification of the standard and unknown species.

In order to develop the calibrations, five standard solutions of a 76 component mixture were prepared in the TNRCC laboratory. Table 3.5 at the end of this section lists the hydrocarbon species used in the calibration mixture. The instrument response was correlated with the concentration for each hydrocarbon species in the standard using linear or polynomial fits, where the correlation coefficient had to be greater than 0.97.

Canister Cleaning

After the canisters were analyzed for their hydrocarbon content, the canisters had to be cleaned and prepared for use again. A cleaning assembly that was designed by the TNRCC and constructed by the University of Texas was used to clean the canisters. Figure 3.5 displays a schematic of the apparatus. The assembly could clean up to 16 cans at one time, over a period of approximately three hours.

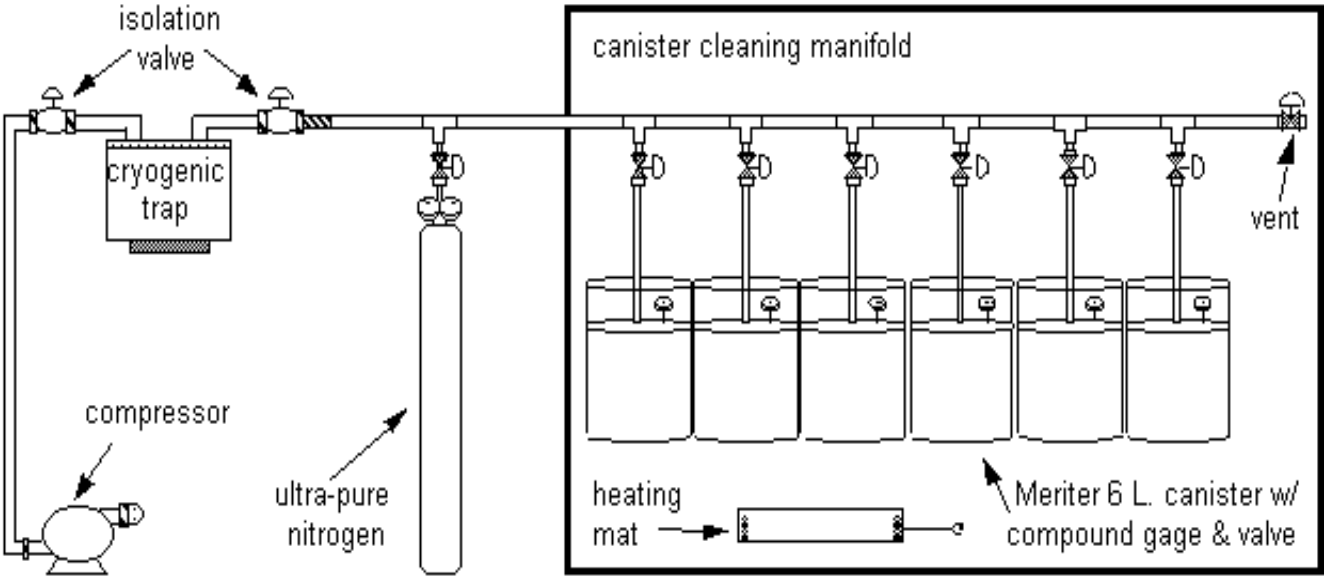


Figure 3.5 Schematic of Canister Cleaning Apparatus (Courtesy of A. Wittig, The University of Texas at Austin)

The cleaning cycle consisted of four separate fill and purge cycles. To prepare for cleaning, the canisters were first emptied of any remaining contents and 100 µL of distilled water was injected into each canister. Next, the canisters were filled with nitrogen gas to 20 psi and heated for approximately five minutes. After heating, the canisters were vented to atmospheric pressure and pumped to 29.4 inches Hg using a Varian SD200 vacuum pump. The second cycle called for filling the canisters to 30psi and then immediately venting to 5psi. In the third cycle, the canisters were filled to 30psi, vented to 5psi, and next vacuumed to 29.4 inches Hg for 20 minutes. The fourth cycle was identical to the third cycle. After the cleaning was complete one of the canisters was chosen for a random clean check on the GC/FID.

Table 3.5 Hydrocarbon species in the calibration mixture for the GC/FID analysis system

RT (min)	Peak ID	Compound	RT (min)	Peak ID	Compound
5.517	4	Propylene	17.067	64	1,1,2-trichloroethane
5.592	5	Propane	17.183	65	2,3,4-trimethylpentane
6.733	7	Isobutane	17.333	66	Toluene
7.375	11	1-butene	17.475	67	2-methylheptane
7.467	11b	1,3-butadiene	17.667	68	3-methylheptane
7.608	12	n-butane	17.817	69	Hexanal
7.917	13	trans-2-butene	18.225	69c	butyl acetate
8.092	14	Bromomethane	18.25	70	n-octane
8.325	16	cis-2-butene	18.442	70b	Tetrachloroethylene
9.483	19	Ethanol	19.217	70c	Chlorobenzene
9.642	20b	2-propenal	19.658	71	Ethylbenzene
9.808	21	Isopentane	19.908	72	p-xylene & m-xylene
9.925	22b	acetone/propanal	20.367	75	Styrene
10.267	23	1-pentene	20.525	76	o-xylene
10.6	24	n-pentane	20.808	77	n-nonane
10.742	25	Isoprene	21.392	79	Isopropylbenzene
10.842	26	trans-2-pentene	22.033	81	benzaldehyde/alpha-pinene
10.933	26b	1,1-dichloroethylene	22.242	83	n-propylbenzene
11.067	27	cis-2-pentene	22.425	83b	p-ethyltoluene
11.217	28	2-methyl-2-butene	22.5	84b	m-ethyltoluene
11.633	30	2,2-dimethylbutane	22.642	85	1,3,5-trimethylbenzene
12.133	31	Cyclopentene	23	86	o-ethyltoluene
12.258	33	4-methyl-1-pentene	23.292	88	beta-pinene
12.442	34	cyclopentane/1,1-dichloroethane	23.45	89	1,2,4-trimethylbenzene
12.525	36	2-methoxy-2-methyl propane	23.692	91	n-decane
12.617	37	2-methylpentane/MTBE	24.35	93	1,2,3-trimethylbenzene
12.767	40	Butanal	25.1	95	m-diethylbenzene
12.958	40b	2-butanone	25.325	96	p-diethylbenzene
13.008	41	3-methylpentane	26.875	98	n-undecane
13.142	43	2-methyl-1-pentene	30.392	99	n-dodecane
13.467	44	n-hexane			
13.6	45	Trans-2-hexene/chloroform			
13.842	46	cis-2-hexene			
14.192	47	Methylcyclopentane/1,2-dichloroethane			
14.417	49	2,4-dimethylpentane			
14.442	51	3-methyl butanal			
14.817	52	benzene			
15.05	54	cyclohexane			
15.192	55	2-methylhexane			
15.258	56	2,3-dimethylpentane			
15.408	57	3-methylhexane			
15.517	57b	1,2-dichloropropane			
15.758	58	2,2,4-trimethylpentane			
16.058	60	n-heptane			
16.558	63	methylcyclohexane			

CHAPTER 4. RESULTS AND DISCUSSION

4.1 Results of the Four Chamber Experiments

Four separate smog chamber experiments were conducted in this study. Table 4.1 below displays a summary of the conditions used in each experiment.

Table 4.1 Summary of Smog Chamber Experiments

Run	*Date*	*Cl_2 injected (cc)*	*Cl_2 injected (ppb_v)*	*Initial NO concen. (ppb_v)*	*Initial TVOC concen. (ppb_c)*	*Max. Temp. (°F)*	*Average Temp. (°F)*
1	10/23/98	30	12	85	980	68	60
2	10/24/98	100	40	90	1400	73	62
3	10/29/98	42	16.5	90	1600	81	75
4	4/6/99	0	0	78	850	82	74

The first three chamber experiments were all conducted in October of 1998. An initial control experiment was also conducted in October of 1998, but due to a problem with the analysis of the VOC canisters, had to be discarded. An additional control experiment was conducted in the spring of 1999. Weather conditions in April were very similar to the conditions in the fall. Appendix A contains all of the solar flux data for each day the smog chamber was run. It includes the global horizontal irradiation, the direct normal irradiation, and the diffuse horizontal irradiation. These data were taken by the solar energy laboratory at the University of Texas at Austin on the main campus at 26th street and Speedway and accessed from their website.[24] Although there are slight fluctuations between each day of the experiments, the solar intensity is relatively similar between runs, and thus neglected as a significant source of error.

RUN 1 OCTOBER 23, 1998

Run 1 was conducted on October 23, 1998 at the Pickle Research Center in Austin, Texas. The smog bag was initially filled with approximately 2500 liters of zero air, five liters of the hydrocarbon mixture (containing 56 different hydrocarbons each at 1 ppm_v in nitrogen), and 10 liters of nitrogen oxide (20.1 ppm_v of NO in nitrogen), and 30 cubic centimeters of chlorine gas (1000 ppm_v in nitrogen). After the smog bag had been mixing for approximately an hour, the first hydrocarbon sample was taken and the bag was then exposed to sunlight at 2:25pm. The high temperature on this day was 68°F and the average was 60°F.[25] The chamber was taken down at 6:15pm after the ozone level had achieved steady state and another hydrocarbon sample was taken. Figure 4.1 shows the results of run 1. Table 4.2 at the end of this section displays a summary of the mass spectrometry analysis of run 1. Appendix B contains the detailed summary from the mass spectrometry analysis.

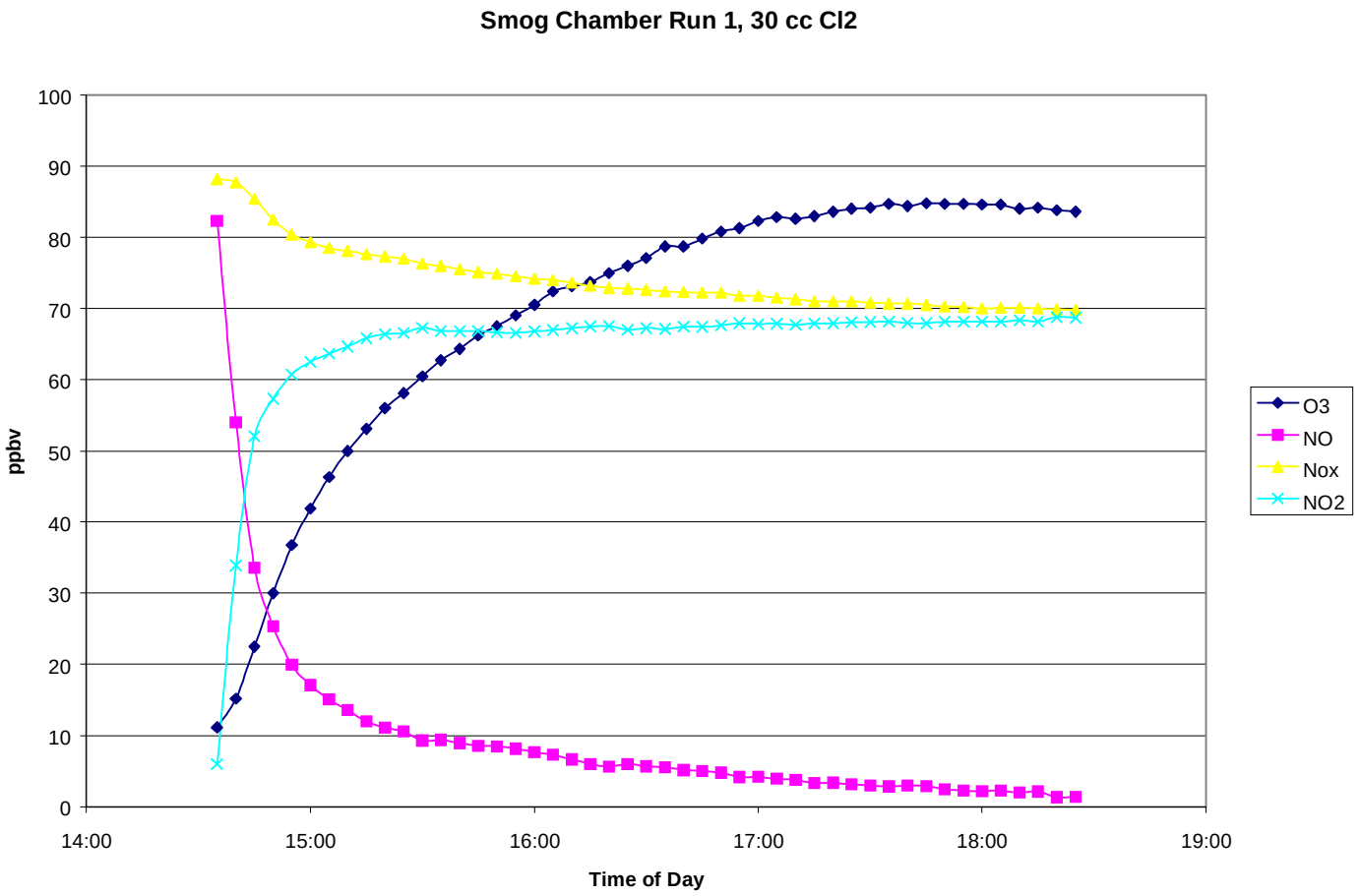


FIGURE 4.1 RESULTS OF SMOG CHAMBER RUN 1

RUN 2, OCTOBER 24, 1998

Run 2 was conducted on October 24, 1998 at the Pickle Research Center in Austin, Texas. The smog bag was initially filled with approximately 2500 liters of zero air, five liters of the hydrocarbon mixture (1ppm$_v$ of 56 different hydrocarbons in nitrogen), and 10 liters of nitrogen oxide (20.1 ppm$_v$ of NO in nitrogen), and 100 cubic centimeters of chlorine gas (1000 ppm$_v$ in nitrogen). After the smog bag had been mixing for approximately an hour, the first hydrocarbon sample was taken and the bag was then exposed to sunlight at 1:15pm. The high temperature on this day was 73°F and the average was 62°F.[25] The chamber was taken down at 5:45pm after the ozone level had achieved steady state and another hydrocarbon sample was taken. Figure 4.2 shows the results of run 2. Table 4.3 at the end of this section displays a summary of the mass spectrometry analysis of run 2. Appendix B contains the detailed summary from the mass spectrometry analysis.

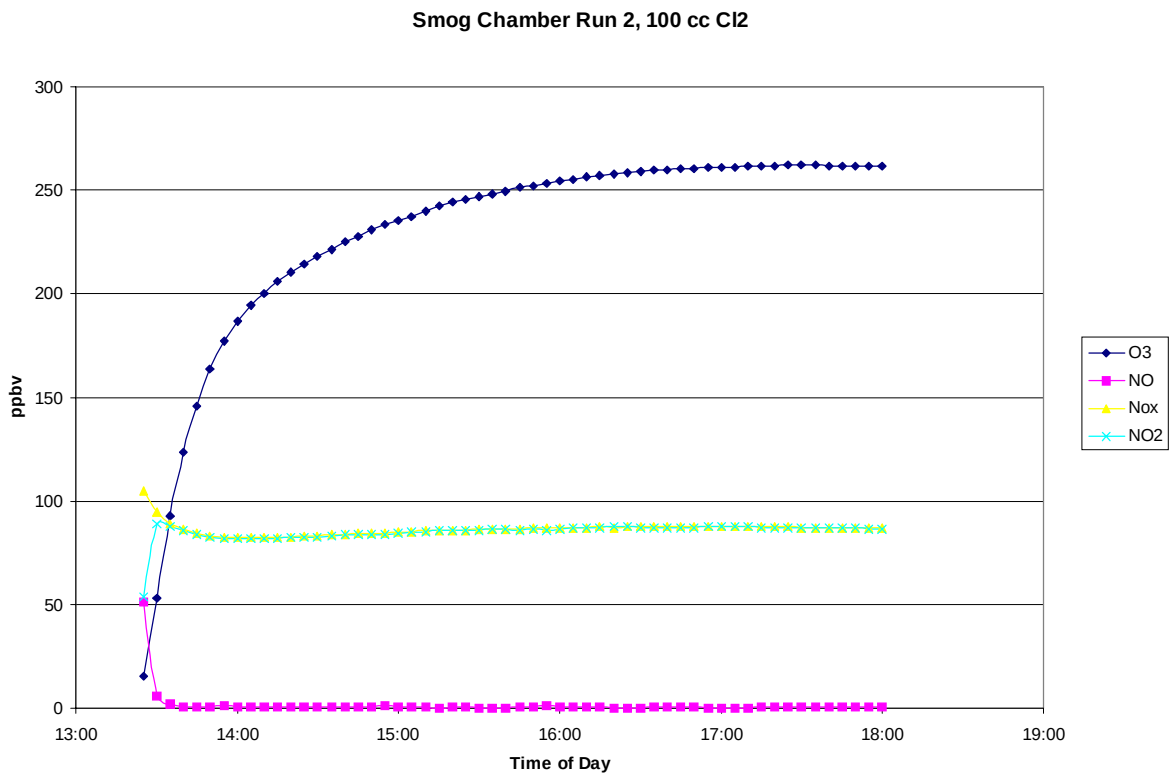


Figure 4.2 Results of Smog Chamber Run 2

RUN 3, OCTOBER 29, 1998

Run 3 was conducted on October 29, 1998 at the Pickle Research Center in Austin, Texas. The smog bag was initially filled with approximately 2500 liters of zero air, five liters of the hydrocarbon mixture (1ppm$_v$ of 56 different hydrocarbons in nitrogen), and 10 liters of nitrogen oxide (20.1 ppm$_v$ of NO in nitrogen), and 42 cubic centimeters of chlorine gas (1000 ppm$_v$ in nitrogen). After the smog bag had been mixing for approximately an hour, the first hydrocarbon sample was taken and the bag was then exposed to sunlight at 1:15pm. The high temperature on this day was 81°F and the average was 69°F.[25] The chamber was taken down at 5:20pm after the ozone level had achieved steady state and another hydrocarbon sample was taken. Figure 4.3 shows the results of run 3. Table 4.4 at the end of this section displays a summary of the mass spectrometry analysis of run 3. Appendix B contains the detailed summary from the mass spectrometry analysis.

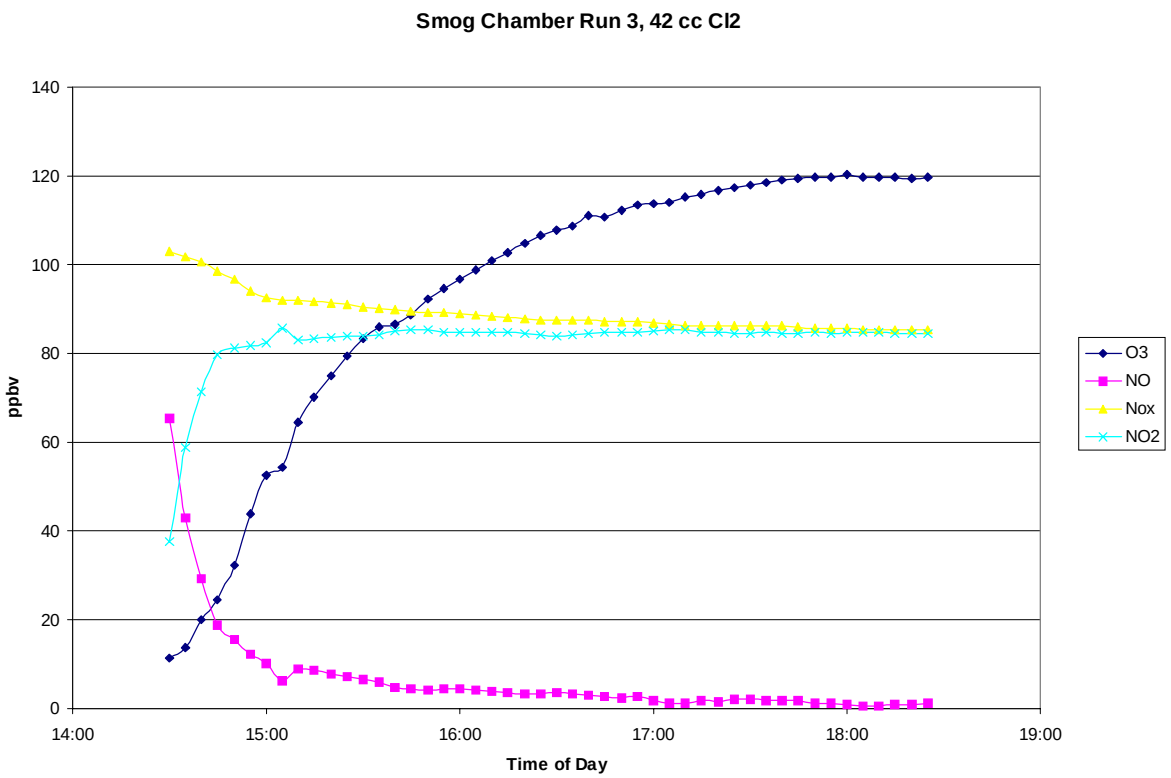


Figure 4.3 Results of Smog Chamber Run 3

RUN 4, APRIL 6, 1999

Run 4 was conducted on April 6, 1999 at the Pickle Research Center in Austin, Texas. The smog bag was initially filled with approximately 2500 liters of zero air, five liters of the hydrocarbon mixture (1ppm$_v$ of 56 different hydrocarbons in nitrogen), and 10 liters of nitrogen oxide (20.1 ppm$_v$ of NO in nitrogen), and no chlorine gas. After the smog bag had been mixing for approximately an hour, the first hydrocarbon sample was taken and the bag was then exposed to sunlight at 12:05pm. The high temperature on this day was 82°F and the average was 74°F.[25] The chamber was taken down at 3:10pm after the ozone level had achieved steady state and another hydrocarbon sample was taken. Figure 4.4 shows the results of run 4. Table 4.5 at the end of this section displays a summary of the mass spectrometry analysis of run 4. Appendix B contains the detailed summary from the mass spectrometry analysis.

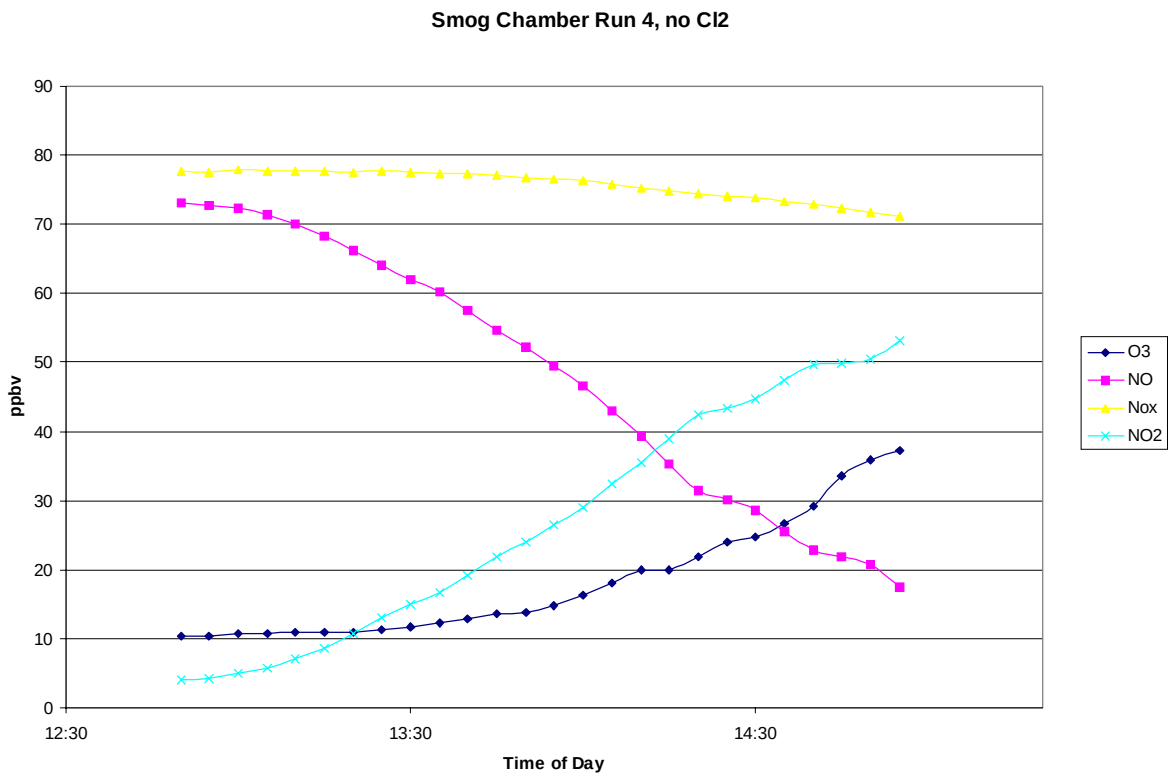
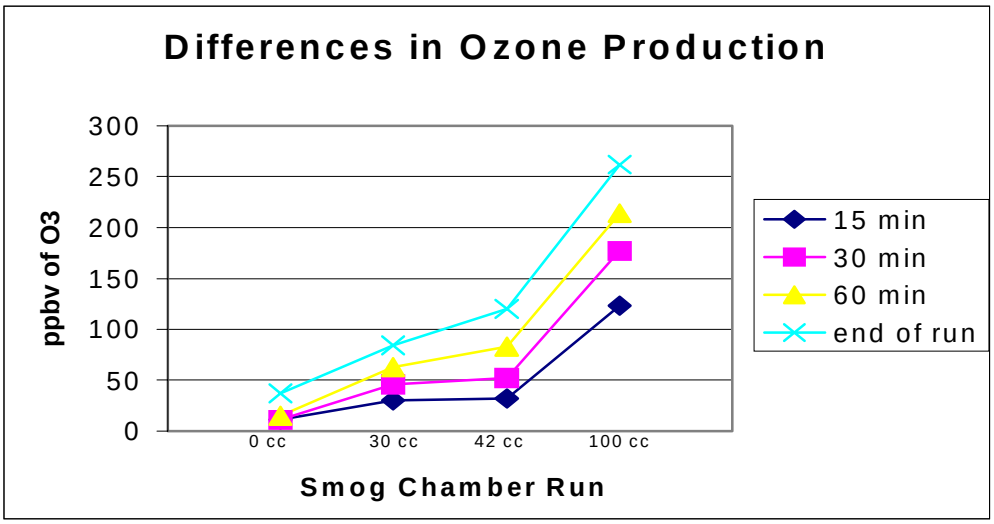


Figure 4.4 Results of Smog Chamber Run 4

OZONE PRODUCTION AS A FUNCTION OF CHLORINE INJECTION

All four of the experiments used approximately the same initial NO_x and hydrocarbon concentrations. Figure 4.5 below displays a summary of the ozone production at varying reaction times and chlorine concentrations.



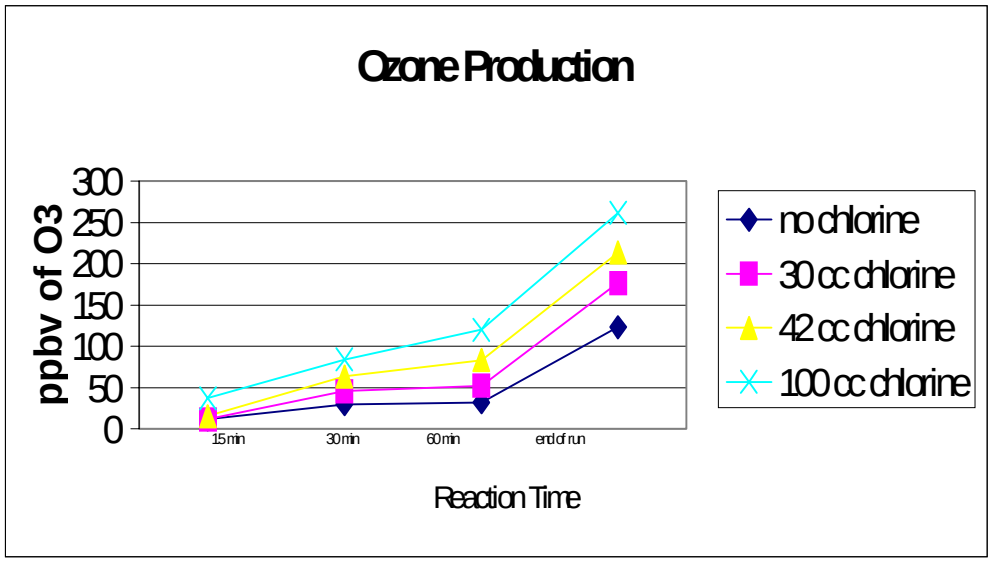


Figure 4.5 Summary of the Difference in Ozone Production

The control experiment that did not receive any chlorine, produced a maximum ozone concentration of approximately 40 ppb_v. As the chlorine concentration increased to 12 ppb_v in the run which used 30 cc of injected Cl_2, the maximum ozone concentration doubled to over 80 ppb_v. As the chlorine increased to 16.5 ppb_v and 40 ppb_v in the runs with 42 cc and 100 cc of Cl_2 injection, the ozone concentration increased dramatically to 120 ppb_v and 260 ppb_v respectively. In each of the experiments the maximum ozone concentration was achieved by the end of the second hour of the experiment. Also interesting to note is $d[O_3]/dt$ as a function of the amount of chlorine injected. The 100 cc run, which utilized 40 ppb_v of chlorine, had accumulated over 100 ppb_v of ozone in the first 15 minutes and 200 ppb_v ozone in the first hour. As the chlorine concentration decreased, so did $d[O_3]/dt$. The 30 cc run, which used 12 ppb_v of chlorine, took about an hour and a half to reach the maximum ozone concentration. Also interesting to note is that runs which had chlorine injected converted all of the NO to NO_2, with d[NO]/dt decreasing as the chlorine concentration increased. The control run however, still had about 15 ppb_v of NO that was never converted to NO_2.

MASS SPECTROMETRY SUMMARIES FROM SMOG CHAMBER RUNS

Tables 4.2 through 4.5 display summaries from the mass spectrometry results. The sample labeled 1-1 refers to run 1 before the smog chamber was exposed to sunlight, while 1-2 refers to run 1 after the experiment was completed. The labels are similar for runs 2 through 4. RT designates retention time, and Qual. is a measure of the confidence level of the compound identification. For the summary tables only those compounds that were identified with a confidence level greater than 70 were chosen to be significant with the exception of a few halogenated compounds. On each of the runs, there were several high molecular weight compounds located between retention times of 25 and 29 minutes. These compounds were tentatively identified as highly fluorinated and highly chlorinated compounds. As seen by the area percentage, these were also very small peaks and thus would usually be deemed as insignificant. However, since these were the only chlorinated (or even possibly chlorinated-due to the low certainty) peaks that were identified in any of the experiments, these peaks seemed as though they could be significant.

Since one of the main of objectives of this study was to find a marker species that could be used to identify chlorine chemistry occurring in ambient conditions, these peaks were closely scrutinized. However, these peaks also occurred in run 4, the control experiment, which had no chlorine gas added. It is believed that these peaks are actually impurities that were released from the teflon bags. A study conducted by Lonnemand et al. also reported that bags made out of FEP teflon film released amounts of volatile residues due to the film manufacturing process.[22] It is not believed however, that these impurities had any affect on the experiment since they were at such low concentrations.

Table 4.2 Summary of Mass Spectrometry Results for Run 1

1-1	1-1	1-1	1-1	1-2	1-2	1-2	1-2
RT	Area%	CMPD	Qual	RT	Area%	CMPD	Qual
3.37*	3.6	Dichlorotetrafluoroethane	58	3.37	3.46	Dichlorotetrafluoroethane	62
6.63	0.14	1,3-Butadiene, 2-methyl	91				
8.53	0.27	Butane, 2,2-dimethyl	53	8.53	0.18	Butane, 2,2-dimethyl	80
9.45	0.21	Cyclopentene	81				
10.02	0.19	1-Pentene	81	10.02	0.11	1-Pentene	72
10.2	0.25	Butane, 2,2-dimethyl					
10.47	0.28	Pentane, 2-methyl	87	10.47	0.16	Pentane, 2-methyl	80
10.78	0.05	Butanal	58	10.8	0.07	Butanal	90
11.17	0.29	Pentane, 3-methyl	72	11.16	0.23	Pentane, 3-methyl	72
11.44	0.22	Cyclohexane	74	11.44	0.02	?	9
12.05	0.31	Hexane	80	12.03	0.16	Hexane	80
12.28	0.25	2-Hexene	87				
12.67	0.25	2-Hexene, <E>	93				
13.14	0.27	Cyclopentane, methyl	87	13.14	0.15	Cyclopentane, methyl	87
13.37	0.35	Pentane, 2,4-dimethyl	87	13.38	0.29	Pentane, 2,4-dimethyl	80
14.13	0.32	Benzene	94	14.14	0.24	Benzene	91
14.48	0.4	Cyclohexane	93	14.48	0.21	Cyclohexane	93
14.85	0.51	Hexane, 2-methyl	90	14.87	0.3	Hexane, 2-methyl	87
14.91	0.47	Pentane, 2,3-dimethyl	91	14.93	0.36	Pentane, 2,3-dimethyl	53
15.17	0.51	Hexane, 3-methyl	81	15.18	0.29	Hexane, 3-methyl	72
15.64	0.68	Heptane, 2,2,4,6,6-pentamethyl	78	15.65	0.44	Heptane, 2,2,4,6,6-pentamethyl	78
15.91*	1.74	Benzene, trifluoromethyl	96	15.92	1.39	Benzene, trifluoromethyl	96
16.01	0.47	Heptane	91	16.02	0.25	Heptane	93
16.7	0.5	Cyclohexane, methyl	96	16.7	0.25	Cyclohexane, methyl	94
17.62	0.62	Pentane, 2,3,4 trimethyl	91	17.62	0.35	Pentane, 2,3,4 trimethyl	86
17.76	0.43	Toluene	95	17.77	0.27	Toluene	93
18.06	0.66	Heptane, 2-methyl	91	18.07	0.37	Heptane, 2-methyl	91
18.99	0.63	Octane	87	18.99	0.31	Octane	90
20.4	0.49	Ethylbenzene	93	20.4	0.29	Ethylbenzene	93
20.64	0.92	p-Xylene	95	20.66	0.37	p-Xylene	95
21.12	0.28	Styrene	95				
21.27	0.47	Benzene, 1,3-dimethyl	95	21.28	0.22	Benzene, 1,3-dimethyl	93
21.63	0.72	Nonane	90	21.64	0.32	Nonane	87
21.92	0.32	Benzene, 1-bromo-3-fluoro	97	21.93	0.24	Benzene, 1-bromo-3-fluoro	97
22.15	0.56	Benzene, 1-methylethyl	95	22.16	0.33	Benzene, 1-methylethyl	95
22.69	0.1	Benzaldehyde	96	22.7	0.06	Benzaldehyde	96
22.75	0.14	alpha pinene	93				
22.97	0.54	Benzene, propyl	91	22.98	0.29	Benzene, propyl-	90
23.19	0.19	Camphene	97				
23.36	0.45	Benzene, 1,3, 5- trimethyl	97				
24.12	0.52	Benzene, 1,2,3 -trimethyl	95	24.13	0.1	Benzene, 1,2,3 -trimethyl	95
25	0.11	Benzene, 1-methy-2-(1-methylethyl)	95				
25.31	0.12	Limonene	95				
25.75	0.07	Acetophenone	94	25.76	0.04	Acetophenone	81
25.93	0.06	Ethane, 1,1,2-trichloro-1,2,2-trifluoro	53	25.95	0.03	Ethane, 1,1,2-trichloro-1,2,2-trifluoro	50
26.85	0.05	Benzene, 1-methyl-4-(1-methylethene)	96				
27.37	0.15	Butane, 1,1,3,4-tetrachloro-1,2,2 trifluoro	64	27.39	0.07	Butane, 1,1,3,4-tetrachloro-1,2,2 trifluoro	38
27.6	0.03	Ethane, 1,1,2-trichloro-1,2,2-trifluoro	59				
28.81	0.02	Butane, trichloroheptafluoroo	38				

Table 4.3 Summary of Mass Spectrometry Results for Run 2

2-1	2-1	2-1	2-1	2-2	2-2	2-2	2-2
RT	Area%	CMPD	Qual	RT	Area %	CMPD	Qual
3.36*	3.49	Dichlorotetrafluoroethane	62	3.37*	1.87	Dichlorotetrafluoroethane	68
				5.54	0.89	Acetone	72
6.64	0.17	1,3-Butadiene, 2-methyl	94				
7.37	0.18	1, Butene, 2- methyl	72				
8.55	0.29	Butane, 2,2-dimethyl	72	8.52	0.22	Butane, 2,2-dimethyl	72
9.46	0.23	Cyclopentene	87				
10.04	0.21	1-Pentene	80	10.02	0.12	1-Pentene	76
10.22	0.28	Butane, 2,3-dimethyl	78	10.19	0.17	Butane, 2,3-dimethyl	80
10.5	0.32	Pentane, 2-methyl	91	10.46	0.17	Pentane, 2-methyl	87
10.78	0.04	Butanal	90	10.78	0.12	Butanal	91
11.21	0.31	Pentane, 3-methyl	87				
11.47	0.24	1-Pentene, 2- methyl	94				
12.05	0.3	Hexane	86	12.01	0.15	Hexane	58
12.28	0.27	2-Hexene	90				
12.68	0.28	2-Hexene, <E>	90				
13.16	0.3	Cyclopentane, methyl	90	13.13	0.13	Cyclopentane, methyl	62
13.37	0.39	Pentane, 2,4-dimethyl	91	13.37	0.2	Pentane, 2,4-dimethyl	64
14.13	0.36	Benzene	94	14.13	0.46	Benzene	94
14.48	0.42	Cyclohexane	91	14.47	0.26	Cyclohexane	81
14.85	0.54	Hexane, 2-methyl	90	14.86	0.26	Hexane, 2-methyl	64
14.91	0.54	Pentane, 2,3-dimethyl	91	14.92	0.42	Pentane, 2,3-dimethyl	47
15.17	0.55	Hexane, 3-methyl	83	15.17	0.3	Hexane, 3-methyl	81
15.64	0.75	Heptane, 2,2,4,6,6-pentamethyl	78	15.65	0.5	Hexane, 2,2-dimethyl	78
15.92*	1.3	Benzene, trifluoromethyl	96	15.93	1.76	Benzene, trifluoromethyl	96
16.01	0.52	Heptane	94	16.01	0.2	Heptane	64
16.7	0.55	Cyclohexane, methyl	96	16.7	0.19	Cyclohexane, methyl	95
17.63	0.69	Pentane, 2,3,4 trimethyl	91	17.63	0.32	Pentane, 2,3,4 trimethyl	72
17.77	0.51	Toluene	97	17.77	0.45	Toluene	95
18.07	0.74	Heptane, 2-methyl	91	18.07	0.32	Heptane, 2-methyl	87
18.29	0.71	Heptane, 3-methyl	90	18.29	0.25	Heptane, 3-methyl	76
18.99	0.7	Octane	94	18.99	0.23	Octane	74
20.41	0.6	Ethylbenzene	94	20.41	0.43	Ethylbenzene	93
20.64	1.14	p-Xylene	97	20.64	0.38	p-Xylene	95
21.12	0.39	Styrene	97				
21.27	0.58	Benzene, 1,3-dimethyl	97	21.28	0.25	Benzene, 1,3-dimethyl	94
21.63	0.84	Nonane	91	21.63	0.21	Nonane	87
21.92	0.24	Benzene, 1-bromo-3-fluoro	94	21.92	0.29	Benzene, 1-bromo-3-fluoro	95
22.15	0.69	Benzene, 1-methylethyl	95	22.15	0.47	Benzene, 1-methylethyl	94
22.71	0.05	Benzaldehyde	96	22.71	0.25	Benzaldehyde	97
22.76	0.23	alpha pinene	93				
22.97	0.68	Benzene, propyl	91	22.97	0.37	Benzene, propyl	91
23.13	0.04	Bicyclo [2.2.1]Heptane, 7,7-dimethyl	98				
23.19	0.26	Camphene	98				
23.36	0.61	Benzene, 1,3, 5- trimethyl	95				
24.12	0.65	Benzene, 1,2,3 -trimethyl	97	24.14	0.09	Benzene, 1,2,3 -trimethyl	86
25	0.15	Benzene, 1-methy-4-(1-methylethyl)	97				
25.31	0.18	Limonene	95				
25.75	0.05	Acetophenone	94	25.76	0.1	Acetophenone	93
25.95	0.05	Ethane, 1,1,2-trichloro-1,2,2-trifluoro	40	25.95	0.07	Ethane, 1,1,2-trichloro-1,2,2-trifluoro	56
26.87	0.07	Benzene, 1-methyl-4-(1-methylethene)	98				
27.36	0.07	Butane, 1,1,3,4-tetrachloro-1,2,2 trifluoro	50				
27.39	0.08	Butane, 1,1,3,4-tetrachloro-1,2,2 trifluoro	53	27.39	0.18	Butane, 1,1,3,4-tetrachloro-1,2,2 trifluoro	38
27.61	0.03	Ethane, 1,1,2-trichloro-1,2,2-trifluoro	59	27.61	0.03	Ethane, 1,1,2-trichloro-1,2,2-trifluoro	38
28.82	0.02	Butane, trichloroheptafluoroo	43				

Table 4.4 Summary of Mass Spectrometry Results for Run 3

3-1`	3-1	3-1	3-1	3-2	3-2	3-2	3-2
RT	Area%	CMPD	Qual	RT	Area%	CMPD	Qual
3.37*	3.53	Dichlorotetrafluoroethane	62	3.37*	3.72	Dichlorotetrafluoroethane	62
				5.56	0.27	Acetone	58
6.64	0.11	1,3-Butadiene, 2-methyl	91				
8.53	0.2	Butane, 2,2-dimethyl	72	8.53	0.16	Butane, 2,2-dimethyl	72
9.46	0.15	Cyclopentene	93				
10.03	0.15	1-Pentene	83	10.02	0.09	1-Pentene	72
10.21	0.2	Butane, 2,3-dimethyl	80	10.19	0.14	Butane, 2,3-dimethyl	80
10.48	0.22	Pentane, 2-methyl	91	10.46	0.13	Pentane, 2-methyl	74
10.76	0.75	Butanal	92	10.79	0.08	Butanal	91
11.46	0.17	1-Pentene, 2- methyl	93				
12.04	0.21	Hexane	58	12.02	0.13	Hexane	64
12.27	0.19	2-Hexene	86				
12.68	0.19	2-Hexene, <E>	93				
13.15	0.21	Cyclopentane, methyl	90	13.14	0.12	Cyclopentane, methyl	83
13.23	0.06	2-Butenal	90				
13.37	0.25	Pentane, 2,4-dimethyl	80	13.37	0.17	Pentane, 2,4-dimethyl	80
14.13	0.24	Benzene	94	14.14	0.25	Benzene	91
14.48	0.31	Cyclohexane	90	14.48	0.17	Cyclohexane	93
14.85	0.38	Hexane, 2-methyl	90	14.86	0.24	Hexane, 2-methyl	64
14.91	0.37	Pentane, 2,3-dimethyl	91	14.92	0.33	Pentane, 2,3-dimethyl	52
15.17	0.41	Hexane, 3-methyl	86	15.17	0.26	Hexane, 3-methyl	74
15.64	0.53	Heptane, 2,2,4,6,6-pentamethyl	78	15.65	0.38	Hexane, 2,2-dimethyl	78
15.92*	1.3	Benzene, trifluoromethyl	96	15.93	1.41	Benzene, trifluoromethyl	96
16.01	0.38	Heptane	93	16.02	0.2	Heptane	93
16.7	0.37	Cyclohexane, methyl	96	16.71	0.19	Cyclohexane, methyl	93
17.63	0.47	Pentane, 2,3,4 trimethyl	91	17.63	0.28	Pentane, 2,3,4 trimethyl	83
17.77	0.33	Toluene	94	17.77	0.28	Toluene	95
18.06	0.74	Heptane, 2-methyl	59	18.07	0.29	Heptane, 2-methyl	87
18.18	0.48	Heptane, 3-methyl	81	18.29	0.29	Heptane, 3-methyl	64
18.99	0.47	Octane	87	18.99	0.25	Octane	87
				19.54	0.01	Cyclopropane, 1-Br-1,2dichloror	4
20.41	0.39	Ethylbenzene	94	20.41	0.28	Ethylbenzene	93
20.64	0.73	p-Xylene	95	20.66	0.33	p-Xylene	94
21.13	0.34	Styrene	94				
21.27	0.38	Benzene, 1,3-dimethyl	97	21.28	0.2	Benzene, 1,3-dimethyl	95
21.64	0.56	Nonane	90	21.63	0.25	Nonane	76
21.93	0.24	Benzene, 1-bromo-3-fluoro	97	21.93	0.25	Benzene, 1-bromo-3-fluoro	95
22.15	0.44	Benzene, 1-methylethyl	95	22.15	0.33	Benzene, 1-methylethyl	94
22.69	0.08	Benzaldehyde	90	22.71	0.2	Benzaldehyde	96
22.76	0.23	alpha pinene	90				
22.97	0.43	Benzene, propyl	91	22.98	0.28	Benzene, propyl	91
23.13	0.04	Bicyclo [2.2.1]Heptane, 7,7-dimethyl	92				
23.19	0.24	Camphene	98				
23.36	0.39	Benzene, 1,3, 5- trimethyl	95	23.38	0.03	Benzene, 1,3, 5- trimethyl	86
24.12	0.42	Benzene, 1,2,3 -trimethyl	95	24.13	0.11	Benzene, 1,2,3 -trimethyl	95
25	0.13	Benzene, 1-methy-4-(1-methylethyl)	97				
25.31	0.17	Limonene	91				
25.75	0.03	Acetophenone	70	25.77	0.05	Acetophenone	81
25.95	0.04	Ethane, 1,1,2-trichloro-1,2,2-trifluoro	72	25.95	0.05	Ethane, 1,1,2-trichloro-1,2,2-trifluoro	53
26.87	0.06	Benzene, 1-methyl-4-(1-methylethene)	96				
27.39	0.12	Butane, 1,1,3,4-tetrachloro-1,2,2 trifluoro	43	27.39	0.12	Butane, 1,1,3,4-tetrachloro-1,2,2 trifluoro	72
27.6	0.02	Ethane, 1,1,2-trichloro-1,2,2-trifluoro	64	27.61	0.02	Ethane, 1,1,2-trichloro-1,2,2-trifluoro	47
28.82	0.02	Butane, trichloroheptafluoroo	53				

Table 4.5 Summary of Mass Spectrometry Results for Run 4

4-1	4-1	4-1	4-1	4-2	4-2	4-2	4-2
RT	Area%	CMPD	Qual	RT	Area %	CMPD	Qual
3.3	2.92	Dichlorotetrafluoroethane	62	3.3	3.33	Dichlorotetrafluoroethane	62
5.16	0.2	Butane, 2-methyl	49	5.16	0.19	Butane, 2-methyl	49
6.46	0.06	1,3-Butadiene, 2-methyl	81				
8.37	0.14	Butane, 2,2-dimethyl	64	8.38	0.14	Butane, 2,2-dimethyl	64
9.31	0.1	Cyclopentene	87				
9.89	0.1	1-Pentene	74	9.98	0.09	1-Pentene	72
10.07	0.14	Butane, 2,3-dimethyl	80	10.06	0.13	Butane, 2,3-dimethyl	72
10.34	0.15	Pentane, 2-methyl	87	10.33	0.13	Pentane, 2-methyl	87
11.05	0.15	Pentane, 3-methyl	80	11.04	0.16	Pentane, 3-methyl	74
11.32	0.1	1-Pentene, 2- methyl	93				
11.92	0.16	Hexane	64	11.91	0.15	Hexane	59
12.16	0.13	2-Hexene	93				
12.56	0.13	2-Hexene, <E>	94				
13.03	0.15	Cyclopentane, methyl	87	13.03	0.13	Cyclopentane, methyl	76
13.26	0.19	Pentane, 2,4-dimethyl	87	13.27	0.17	Pentane, 2,4-dimethyl	87
14.02	0.13	Benzene	93	14.03	0.14	Benzene	93
14.37	0.2	Cyclohexane	93	14.37	0.17	Cyclohexane	81
14.76	0.26	Hexane, 2-methyl	83	14.76	0.23	Hexane, 2-methyl	87
14.81	0.23	Pentane, 2,3-dimethyl	90	14.82	0.25	Pentane, 2,3-dimethyl	87
15.07	0.25	Hexane, 3-methyl	93	15.07	0.22	Hexane, 3-methyl	93
15.54	0.34	Pentane, 2,2,4-trimethyl	64	15.54	0.33	Hexane, 2,2-dimethyl	53
15.82	0.63	Benzene, trifluoromethyl	97	115.83	0.63	Benzene, trifluoromethyl	96
15.91	0.25	Heptane	93	15.92	0.22	Heptane	93
16.61	0.26	Cyclohexane, methyl	96	16.6	0.21	Cyclohexane, methyl	96
17.53	0.32	Pentane, 2,3,4 trimethyl	91	17.53	0.28	Pentane, 2,3,4 trimethyl	91
17.67	0.26	Toluene	93	17.67	0.23	Toluene	93
17.97	0.35	Heptane, 2-methyl	91	17.97	0.29	Heptane, 2-methyl	90
18.19	0.33	Heptane, 3-methyl	90	18.19	0.28	Heptane, 3-methyl	87
18.9	0.34	Octane	93	18.9	0.29	Octane	93
20.31	0.3	Ethylbenzene	93	20.3	0.26	Ethylbenzene	93
20.55	0.53	Benzene, 1,3-dimethyl	94	20.55	0.37	Benzene, 1,3-dimethyl	95
21.17	0.27	Benzene, 1,2-dimethyl	94	21.17	0.21	Benzene, 1,2-dimethyl	94
21.54	0.4	Nonane	93	21.53	0.32	Nonane	94
x	x	Benzene, 1-bromo-3-fluoro	x	x	x	Benzene, 1-bromo-3-fluoro	x
22.04	0.28	b	93	22.04	0.28	Benzene, 1-methylethyl	93
22.86	0.29	Benzene, propyl	94	22.86	0.28	Benzene, propyl-	91
23.26	0.03	Benzene, 1,3, 5- trimethyl	55	23.25	0.04	Benzene, 1,3, 5- trimethyl	92
24.01	0.08	Benzene, 1,2,3 -trimethyl	94	24.01	0.1	Benzene, 1,2,3 -trimethyl	95
25.82	0.02	Ethane, 1,1,2-trichloro-1,2,2-trifluoro	37	25.82	0.01	Ethane, 1,1,2-trichloro-1,2,2-trifluoro	47
27.26	0.1	Butane, 1,1,3,4-tetrachloro-1,2,2 trifluoro	50	27.23	0.03	Butane, 1,1,3,4-tetrachloro-1,2,2 trifluoro	47
27.48	0.02	Ethane, 1,1,2-trichloro-1,2,2-trifluoro	43	27.26	0.03	Ethane, 1,1,2-trichloro-1,2,2-trifluoro	25
28.68	0.02	Butane, trichloroheptafluoroo	43	27.48	0.01	Butane, trichloroheptafluoroo	43

4.2 Relative Reactivities of Hydrocarbons

A representative set of hydrocarbons from the results of the mass spectrometry was chosen for detailed analysis. The compounds chosen were: an alkane, a substituted alkane, an olefin, a substituted olefin, an aromatic, and a substituted aromatic. Specifically, the VOCs chosen were hexane, 2,3-dimethyl pentane, 1-pentene, isoprene, benzene, and toluene. As discussed in section 2.4 these compounds react at very different rates with hydroxyl radicals than with chlorine radicals. Thus, it is expected that the concentrations of the representative set of hydrocarbons in the presence of Cl_2 will differ from the concentrations when oxidation reactions are dominated by hydroxyl radicals.

Hydroxyl radical attack is the most important reaction pathway for most compounds in the ozone formation chemistry, while chlorine radical attack dominates for the hydrocarbons which react slowly with the hydroxyl radicals (alkanes and substituted alkanes). By examining the concentrations of hydrocarbons before and after the smog chamber experiments run it is possible to see how chlorine affects the concentrations of the VOCs. Tables 4.6 through 4.9 display the concentrations of hydrocarbons. Results are given in parts per billion volume (ppb_v) and parts per billion carbon (ppb_C). Headings 1-1, 2-1, 3-1, and 4-1 refer to runs 1, 2, 3, and 4 respectively, before the chamber was exposed to sunlight, while headings 1-2, 2-2, 3-2, and 4-2 refer to runs 1, 2, 3, and 4, respectively after each experiment was completed. Also included in these summaries are several additional alkanes, octane and nonane, since these are the compounds that differed the most from the control experiment (no chlorine injected).

Table 4.6 Hydrocarbon Concentration Results for Run 1, 12 ppbv Cl_2 added

1-1	1-1	1-1	1-2	1-2	1-2
	ppbv	ppbC		pbbv	ppbC
1,3-Butadiene, 2-methyl	2.2	11.2	1,3-Butadiene, 2-methyl	0	0
1-Pentene	2.1	10.7	1-Pentene	1.6	7.8
Hexane	2.3	13.5	Hexane	1.4	8.7
Benzene	2.3	14	Benzene	2.3	13.9
Pentane, 2,3-dimethyl	2	14.2	Pentane, 2,3-dimethyl	1.4	10
Toluene	2	14.1	Toluene	1.8	12.4
Octane	1.9	15.1	Octane	1.3	10.1
Nonane	2.1	19.2	Nonane	1	9

Table 4.7 Hydrocarbon Concentration Results for Run 2, 40 ppbv Cl_2 added

2-1	2-1	2-1	2-2	2-2	2-2
	ppbv	ppbC		pbbv	ppbC
1,3-Butadiene, 2-methyl	2.3	11.3	1,3-Butadiene, 2-methyl	0	0
1-Pentene	3.1	15.4	1-Pentene	2.1	10.3
Hexane	3	18	Hexane	1.2	7.1
Benzene	3.7	22.2	Benzene	3.3	19.9
Pentane, 2,3-dimethyl	3	21.3	Pentane, 2,3-dimethyl	1.1	7.7
Toluene	3.3	22.9	Toluene	2.6	18.4
Octane	2.9	23.2	Octane	0.7	5.7
Nonane	3	27.3	Nonane	1.7	15.3

Table 4.8 Hydrocarbon Concentration Results for Run 3, 16.5 ppbv Cl_2 added

3-1	3-1	3-1	3-2	3-2	3-2
	ppbv	ppbC		pbbv	ppbC
1,3-Butadiene, 2-methyl	2.1	10.6	1,3-Butadiene, 2-methyl	0	0
1-Pentene	2.2	10.8	1-Pentene	1.5	7.3
Hexane	1.9	11.5	Hexane	1.2	7.2
Benzene	2.3	13.6	Benzene	2.3	13.6
Pentane, 2,3-dimethyl	2.9	20.4	Pentane, 2,3-dimethyl	1.1	7.7
Toluene	1.9	13.6	Toluene	1.9	13.5
Octane	2	16.1	Octane	0.9	7.6
Nonane	2.1	21.6	Nonane	1.2	10.6

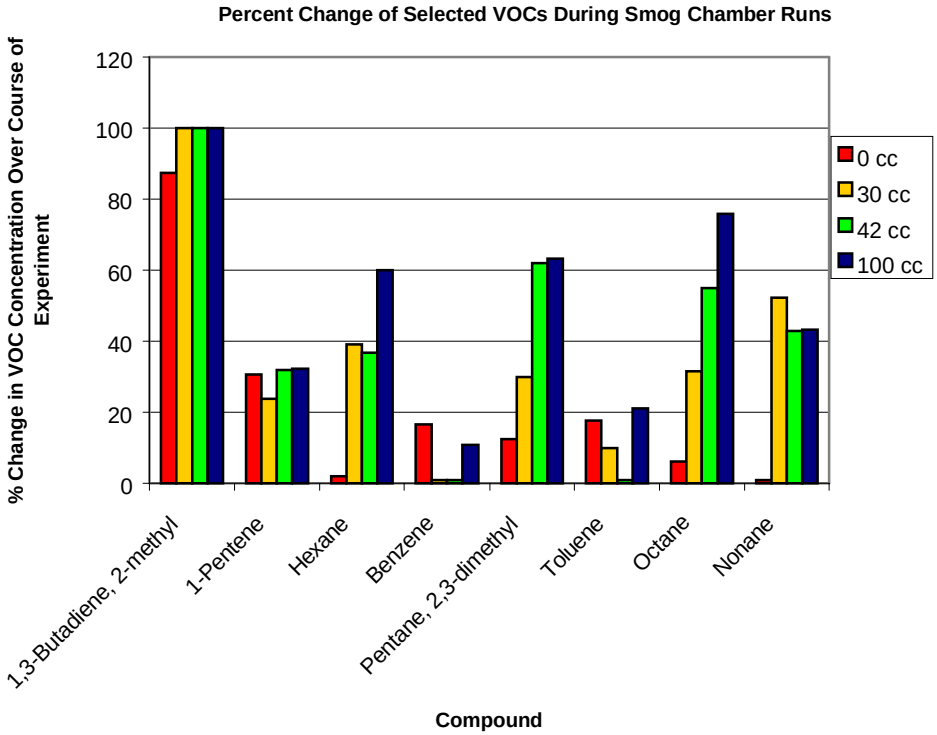


Figure 4.6 Percent Change of Selected VOCs During Smog Chamber Runs

Table 4.9 Hydrocarbon Concentration Results for Run 4, no Cl_2 added

4-1	4-1	4-1	4-2	4-2	4-2
	ppbv	ppbC		pbbv	ppbC
1,3-Butadiene, 2-methyl	1.6	8	1,3-Butadiene, 2-methyl	0.2	1.1
1-Pentene	2.6	13	1-Pentene	1.8	8.8
Hexane	1.7	10.4	Hexane	1.7	10.1
Benzene	1.8	10.7	Benzene	1.5	9.2
Pentane, 2,3-dimethyl	1.6	11.5	Pentane, 2,3-dimethyl	1.4	10.1
Toluene	1.7	12	Toluene	1.4	10.1
Octane	1.6	13.1	Octane	1.5	12
Nonane	2.4	21.5	Nonane	2.4	21.5

Figure 4.6 below displays the percent change in concentration from before the chamber was run until the experiment was completed for each one of the compounds, for each run.

It is apparent from Figure 4.6 that alkanes and substituted alkanes reacted more extensively in the runs that had chlorine injections than in the blank run. Isoprene (1,3-butadiene, 2-methyl) reacted almost completely for all four runs, as expected. Approximately 30% of the 1-pentene reacted for all four runs, showing little impact from the addition of chlorine. However hexane, 2,3-dimethyl pentane, octane, and nonane all showed significant reactivity for the runs that had chlorine injection. Benzene and toluene concentrations were not influenced by chlorine injection. All of the results seemed to show what was expected, that the chlorine would significantly alter the reaction rates of the alkanes and substituted alkanes, and not affect the rest of the VOCs. Appendix C contains the complete FID results for all of the compounds that were analyzed.

4.3 Identification of Marker Species

One of the main objectives of this project was to identify a hydrocarbon marker(s) species that can assist in identifying whether chlorine reactions are significant. It was hypothesized that a chlorinated hydrocarbon would appear in the mass spectrometry analysis as a product of the chlorine chemistry. This compound, if found in an ambient air sample, could then be an indicator of chlorine chemistry in the marine boundary layer or near an anthropogenic source of chlorine. However, no such species were found in the analysis. Chlorine atoms react with the hydrocarbons, abstracting hydrogen to form hydrogen chloride (HCl) almost exclusively. The only chlorinated peaks that were identified were believed to be due to impurities released from the bag. This is shown since run 4, which did not use any chlorine, also contained these peaks in the mass spectrometry results.

Although no specific hydrocarbon marker species were identified, chlorine reactions in ambient air can be identified by low ratios of alkanes to the other reactive hydrocarbons. As discussed in the previous section, the reactivity of alkanes is significantly different when chlorine is injected than in the control run. An air mass that has had significant chlorine reactions should have a much higher percentage of its alkanes and substituted alkanes reacted than a typical urban air mass.

4.4 Analysis of Ambient Data from Houston

In the greater Houston area there are several anthropogenic sources of chlorine emissions. In 1993, the largest such emitter released approximately 16 million pounds of chlorine in 1993 through a continuous stack release.[13] Figure 4.7 shows the location of the three largest chlorine sources in Houston (represented by triangles) as well as the Clinton and Aldine air quality monitoring sites.

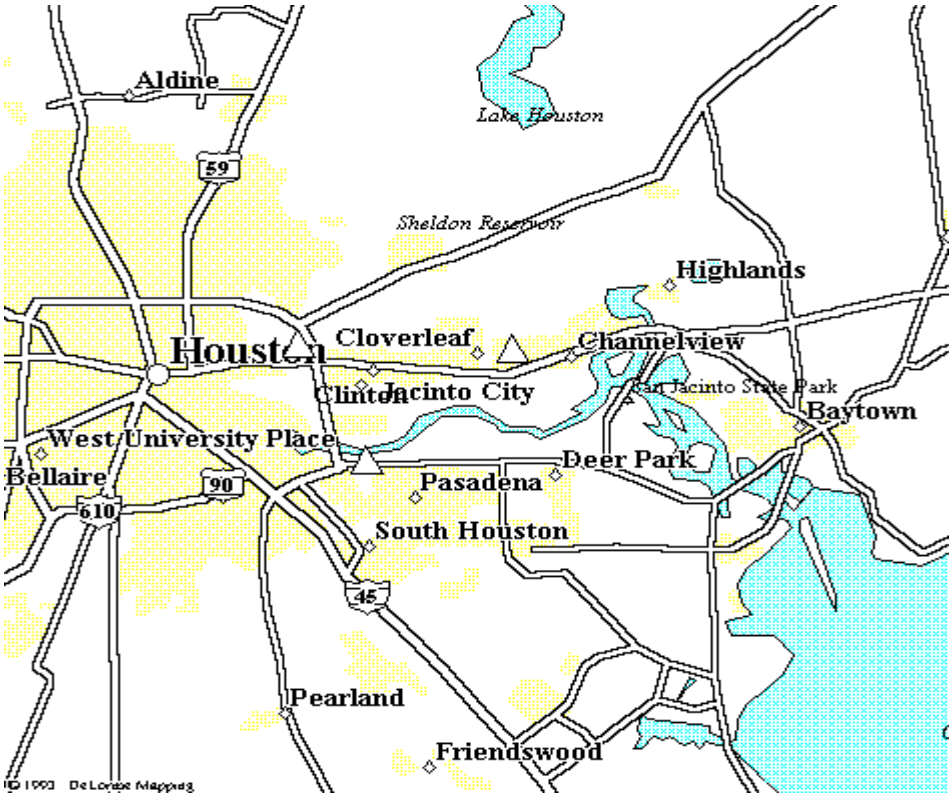


Figure 4.7 Locations of the Chlorine Sources in Relation to Monitoring Sites

On August 19, 1993 there was an unexplained ozone spike at the Aldine monitoring site. Surrounding monitoring sites like Clinton, which normally record maximum ozone concentrations similar to those observed at Aldine, all observed maximum afternoon ozone concentrations of approximately 160 ppbv. The Aldine site, however, had a maximum ozone concentration of 244 ppbv. Figure 4.8 below displays the observed ozone concentrations for August 19, 1993. The Clinton site is abbreviated by C35C and the Aldine site is abbreviated by HALC. The remaining symbols correspond to monitoring sites around the Houston area. They are all also significantly lower than the Aldine reading.

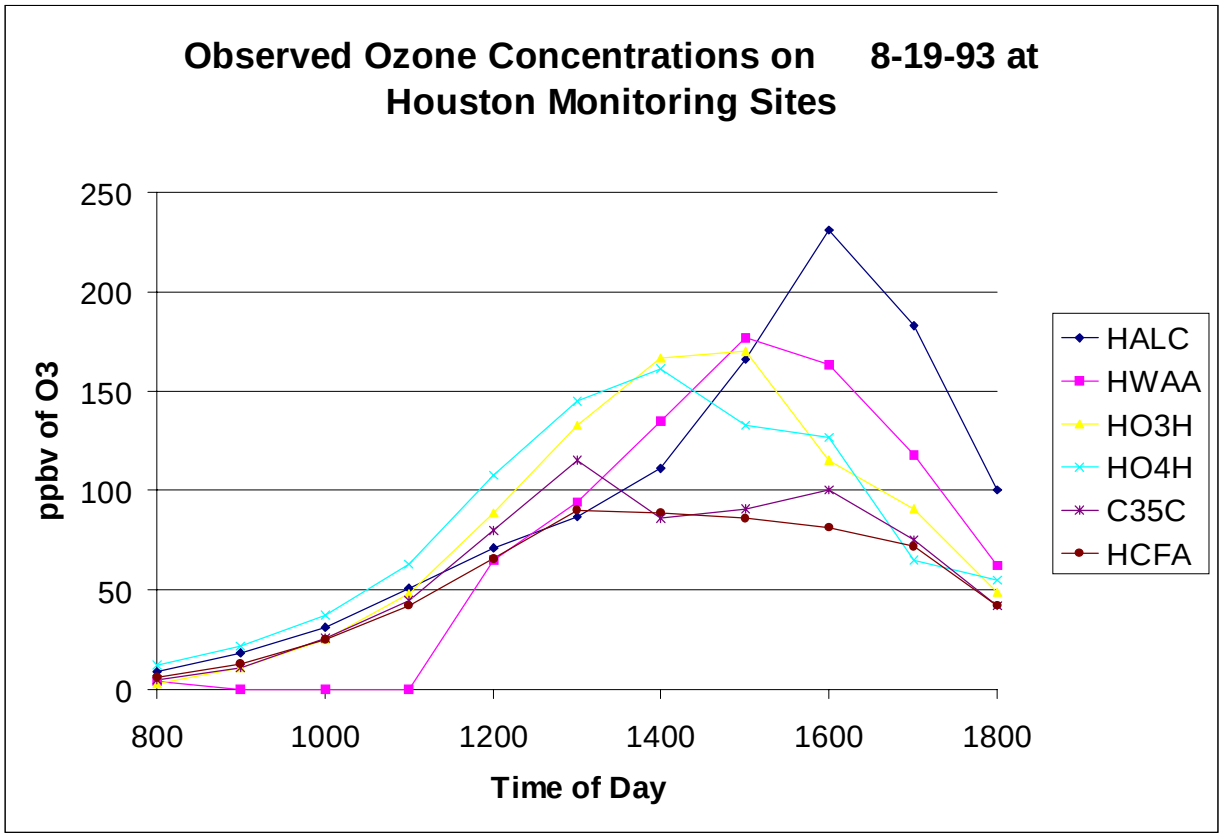


Figure 4.8 Observed O_3 Concentration in the Houston Area on 8-19-93

The back trajectory for the air parcel arriving at Aldine on this day, obtained from Dr. Neece at TNRCC, is shown in Figure 4.9. This is a very unusual trajectory for this area. The trajectory begins at 8:00 am at point 0 on the map and ends at the local maximum ozone production. As shown, the air parcel originated south of Harris County, traveled out toward the ship channel, and then turned course back towards Houston. It then passed over the Clinton monitoring site and next over the chlorine sources. The air parcel then ended at the Aldine site, which was the local maximum ozone concentration. There is approximately a 3 hour delay from Clinton until the air parcel reaches Aldine. Thus, August 19, 1993 gives a unique opportunity to view what happens when an air parcel travels over Houston, passes over an monitoring site (Clinton), receives a chlorine injection, and then passes over a monitoring site again.

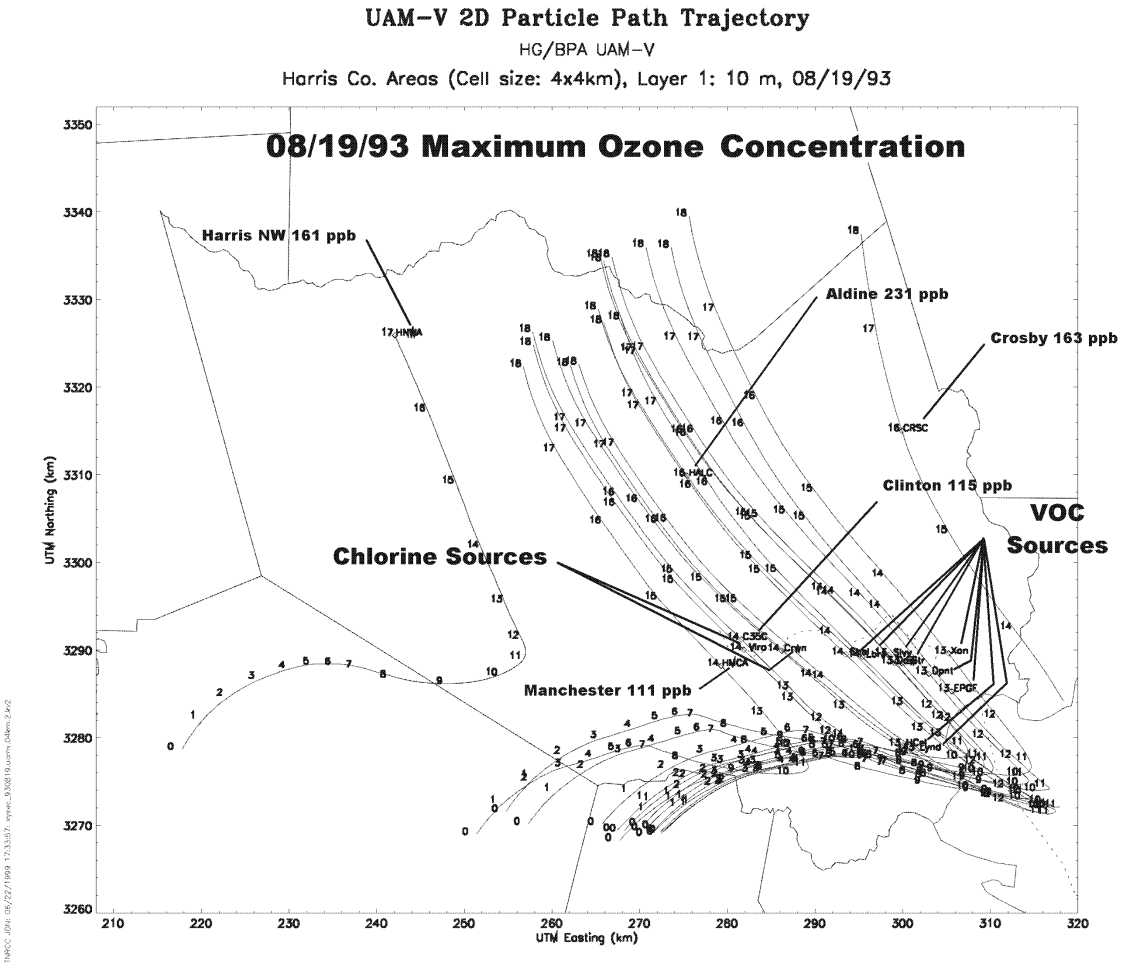


Figure 4.9 Back Trajectory of the Houston region for 8-19-93

The Clinton and Aldine monitoring sites both have VOC canister data from August 19, 1993. Figures 4.10 and 4.11 located at the end of the section show the concentrations of a representative set of hydrocarbons from the Aldine and Clinton sites on August 19, 1993. The times represented on the "y-axis" correspond to a 24 hour clock (for example 14 represents 2:00 pm). Table 4.10 below gives an explanation of the VOC abbreviations for all of the charts in this section.

Table 4.10 Explanation of Abbreviations for VOCs

FIELD_NAME	EXPL
APINEN	alpha-pinene
BENZE	benzene
BZ124M	1,2,4-trimethylbenzene
BZ135M	1,3,5-trimethylbenzene
CYHEXA	cyclohexane
ETHANE	ethane
ETHENE	ethene
HEP22D	2,2-dimethylheptane
HEP2ME	2-methyl heptane
HEXA3M	3-methylhexane
IPENTA	isopentane
I_BUBZ	isobutylbenzene
I_BUTA	isobutane
MP_XYL	mp-xylene
M_ETOL	m-ethyltoluene
N_BUTA	n-butane
N_DEC	n-decane
N_HEPT	n-heptane
N_HEX	n-hexane
N_OCT	n-octane
N_PROP	n-propane
N_PENT	n-pentane
PA224M	2,2,4-trimethylpentane
PEN23M	2,3-dimethylpentane
PENA2M	2-methylpentane
PENA3M	3-methylpentane
PENTE1	1-pentene
PROPE	Propene
TOLUE	toluene

Since there is approximately a 2 to 3 hour delay from the Clinton data to the Aldine data, the VOCs that are shown at 11 (11:00 am) for Clinton arrive at Aldine at approximately 14 (2:00 pm). There is an abnormally high release of parafins (for example 2,3-dimethyl pentane at 11) evident in the Clinton data. This paraffin plume has been noted in the Clinton data previously and although not a daily release, such events are not uncommon in Houston. [26] It is most likely due to an abnormal release or an upset in an industrial source somewhere along the back trajectory. Such releases are not uncommon in Houston, and usually will not produce an ozone

spike alone since the hydroxyl radical reaction with paraffins is relatively slow. To further demonstrate what is occuring, a broader set of VOCs are displayed for Clinton at 11 and Aldine at 14 in figures 4.12 and 4.13 located at the end of the section. These compounds were chosen from the entire set of identified compounds as ones that had concentrations above 5 ppb_C, or they were chosen if they were part of the representative set of compounds studied in the smog chamber studies. Once again, due to the delay in the back trajectory, these times represent the same air parcel as it moves along.

The first major observation when comparing the speciation of the air parcel when it is at Clinton at 11 and when it reaches Aldine at 14 is the disapperance of the paraffin plume. The unusually large amount of 2,3-dimethyl pentane which was over 40 ppb_C at Clinton is reduced to a trace amount by the time the air parcel reaches Aldine at 14. While almost all the compounds were significantly reduced, the parrafins, which usually display little reactivity in typical smog chemistry, are significantly more reacted than the rest of the VOCs.

Our hypothesis is that this unusual chemistry can best be explained by the air parcel's interaction with chlorine. As discussed previously, the back trajectory for August 19, 1993 was not a typical day. The air parcel passed over Houston and many industrial sources accumulating high concentrations of many VOCs. It then passed over the Clinton monitoring site before passing a chlorine source where it received a chlorine injection. If this ambient air mass behaved similarly to the controlled reactions in the smog chamber, then two major events should have occurred. First, there should have been a dramatic increase in ozone production depending on the exact chlorine concentration in the air mass. Second, the chlorine chemistry in the air mass would be evidenced by the disappearance of alkanes and subsituted alkanes. If these paraffins reacted at significantly greater levels than usual, then this is an indicator of chlorine interaction in an ambient urban air mass.

Both of these events did occur. The projected maximum ozone concentration for Aldine was approximately 160 ppb, comparable to all of the other monitoring sites in the greater Houston area. However it reached an afternoon maximum of 244 ppb. In addition, the paraffins in the Aldine data did react at significantly greater rate than usual and in comparison to the rest of the compounds. Finally, there seemed to be an unusually high amount of parrafins released on August 19, 1993. So instead of having an ambient mass with similar concentrations of all of the VOCs, the air parcel which traveled over the the chlorine source was concentrated in alkanes and substituted alkanes. While emergency releases are relatively common, it was the combination of these events that caused the unexplained ozone spike at Aldine on August 19, 1993. The chlorine from the industrial facility is a continuous stack release, and the upsets are common, but the ozone spikes only occur when there is the appropriate back trajectory where they mix.

The ozone peaked at Aldine just after 16 (1600 hr), but the last VOC measurement taken at either of the sites was at 14 (1400 hr). So while there are no hydrocarbon data to illustrate what compounds had reacted at the peak time, the 14 data from Clinton can be used to show what VOCs the air parcel contained when it arrived at Aldine during the ozone spike. Figure 4.14 at the end of the section shows the data from the Clinton site at 14 which arrived in Aldine approximately around the time of the maximum ozone concentration. Most of the compounds appear to be at similar levels as the 11 (11:00 am) data, except for a large amount of 2,2-dimethyl heptane , 1,2,4-trimethyl benzene, and isobutylbenzene. Although there is not definitive data from Aldine at 18 (6:00 pm), around the time of the spike, if the air parcel behaves similarly to the previous one discussed then the large amount of 2,2-dimethyl heptane should have significantly reacted, causing the unusual ozone spike on August 19, 1993.

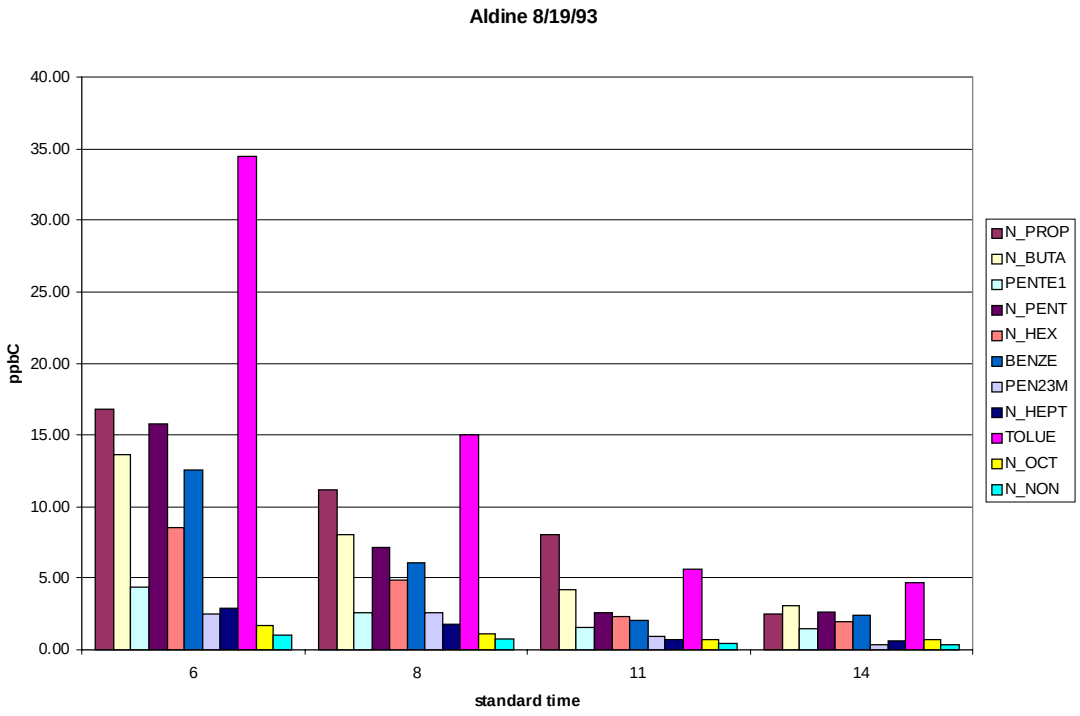


Figure 4.10 Selected Set of VOCs for Aldine on 8-19-93

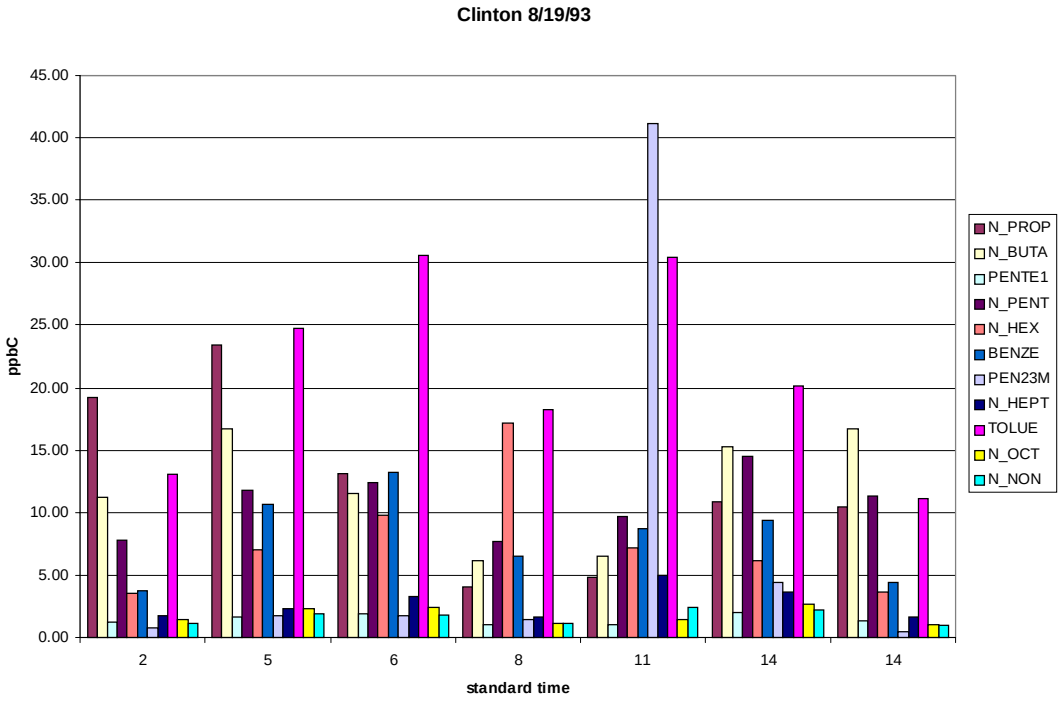


Figure 4.11 Selected Set of Hydrocarbons for Clinton on 8-19-93

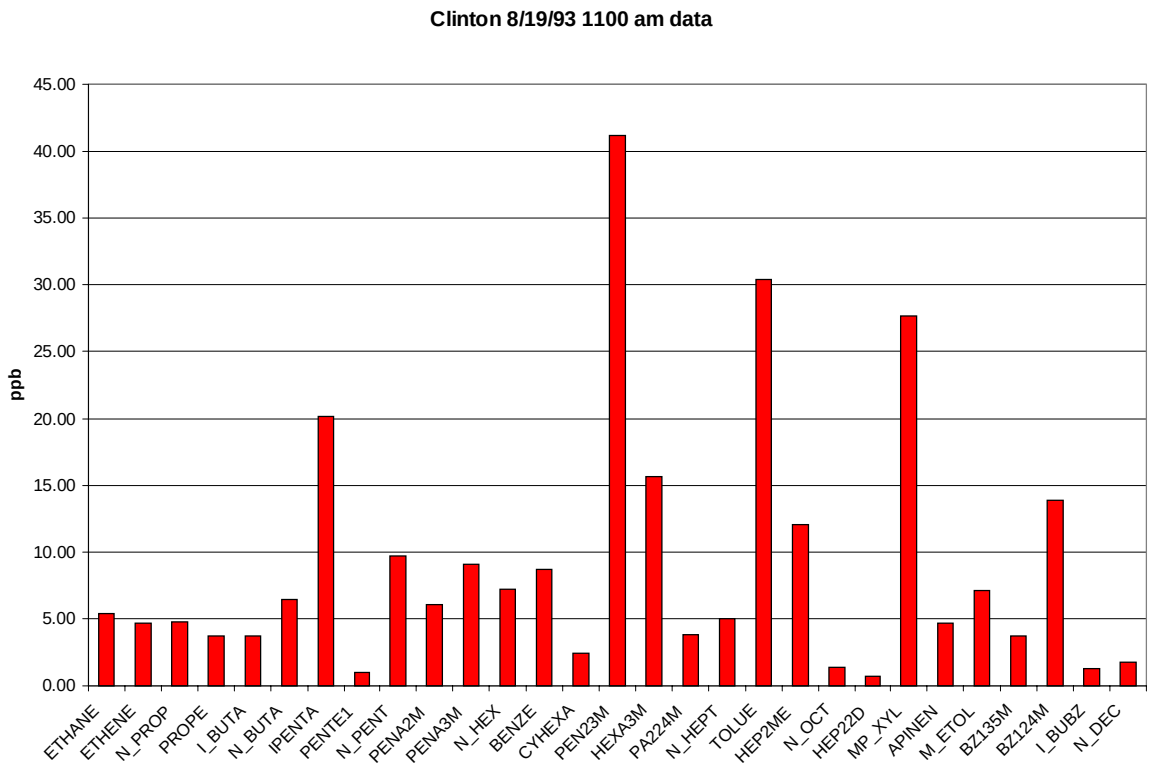


Figure 4.12 Broad Set of VOCs for Clinton at 11:00 am on 8-19-93

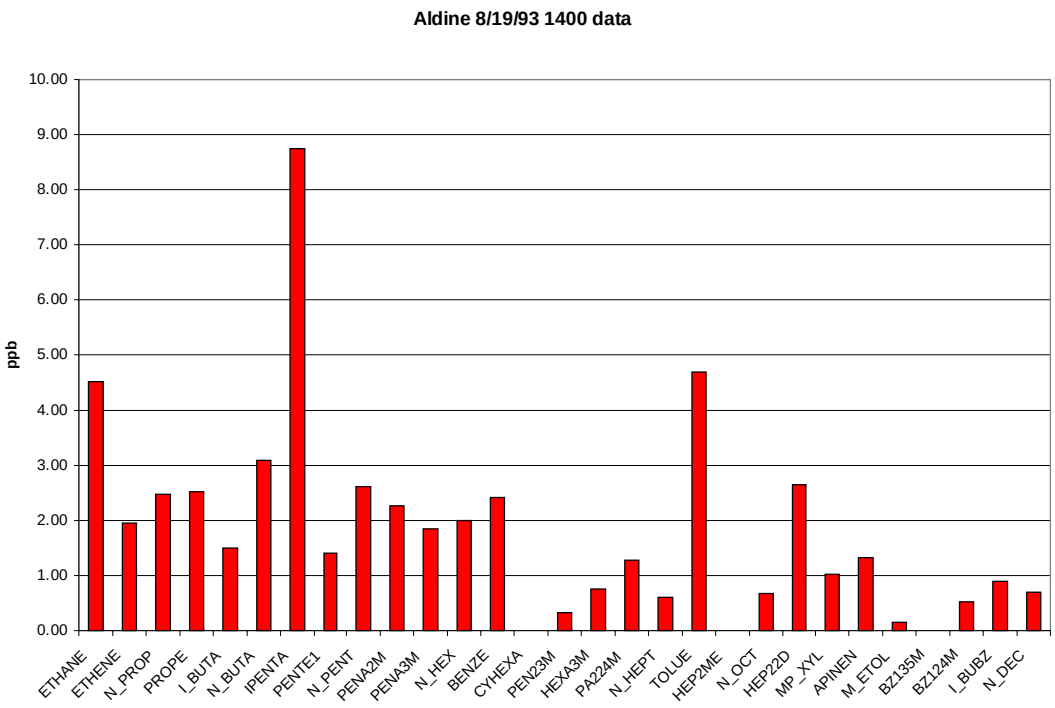


Figure 4.13 Broad Set of VOCs for Aldine at 2:00 pm on 8-19-93

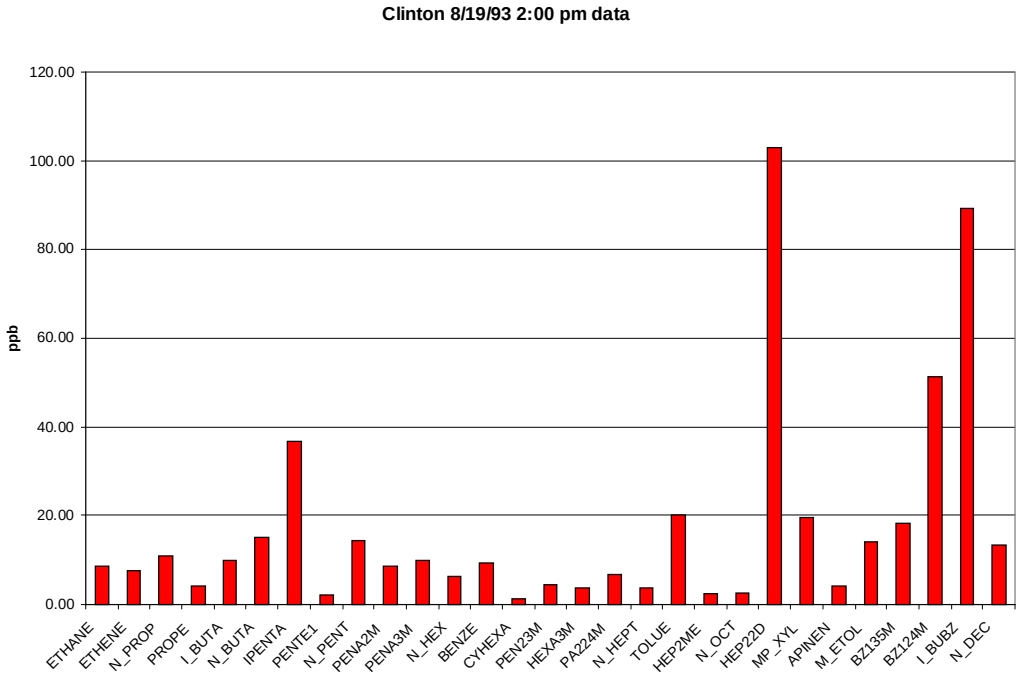


Figure 4.14 Broad Set of VOCs for Clinton at 2:00 pm on 8-19-93

CHAPTER 5. SUMMARY

The objective of this project was to study the role of chlorine in affecting ozone formation chemistry. Preliminary studies have indicated that such chlorine can significantly affect the photochemistry of ozone formation. Specifically, there were three major objectives:

1. determine the effect of molecular chlorine on the kinetics of ozone formation in a mixture representing the atmosphere of a coastal urban center
2. identify hydrocarbon marker species that can assist in characterizing the extent of chlorine reactions
3. examine ambient air quality data from Southeast Texas for evidence of chlorine chemistry

A series of four separate smog chamber experiments were conducted to meet these objectives. Table 5.1 below summarizes the results of these experiments.

Table 5.1 Summary of Results from Smog Chamber Experiments

Cl_2 Injected (cc)	Cl_2 injected (ppb_v)	Initial NO (ppb_v)	Initial Analyzed TVOC (ppb_C)	O_3 Maximum ($ppb_{v)}$
0	0	78	850	40
30	12	85	980	83
42	16.5	90	1600	120
100	40	90	1400	262

It is evident that the injection of chlorine into the simulated air mass in the smog chamber resulted in a dramatic increase in ozone production. The control run in which no chlorine was injected, only produced 40 ppb_v of ozone. However, the experiments with chlorine injections had maximum ozone concentrations that ranged from 83 to 262 ppb_v. The effects of chlorine on ozone production were rapid, occurring in approximately the first 15 minutes.

Another one of the objectives of the experiment was to find hydrocarbon marker species that can assist in identifying when chlorine reactions occur. While no chlorinated marker species could be found, the relative reactivities of volatile organic compounds can be used to determine if chlorine chemistry is significant. The alkanes and substituted alkanes, which typically do not react significantly with hydroxyl radicals, reacted to a significant extent when chlorine was injected. The concentrations of olefins and aromatics remained unchanged between the experiments with chlorine and without injection. Thus, decreased concentrations of alkanes in ambient air samples could serve as an indicator that chlorine chemistry is occurring.

The results of the chamber experiments were used to assess the potential impact of chlorine chemistry for an August 19, 1993 episode. The observations for this episode were consistent with the chemistry observed in the chamber experiments, suggesting that chlorine may play a significant role in some ozone episodes.

Appendix A

Solar Radiation Data

DAY = Julian day
GHI = Global Horizontal Irradiation
DNI = Direct Normal Irradiation
DHI = Diffuse Horizontal Irradiation
TEMP = Temperature

23RD OCTOBER 1998

YEAR	DAY	TIME	GHI	DNI	DHI	TEMP
1998	296	1200	775	980	60.91	17.82
1998	296	1205	775	978	59.6	17.68
1998	296	1210	776	979	59.97	17.84
1998	296	1215	779	984	60.05	18.17
1998	296	1220	777	977	56.69	17.61
1998	296	1225	777	979	58.2	17.33
1998	296	1230	776	980	58.77	17.6
1998	296	1235	776	980	57.42	17.65
1998	296	1240	773	979	59.23	17.92
1998	296	1245	769	977	58.75	17.97
1998	296	1250	767	976	56.96	17.99
1998	296	1255	765	975	56.72	18.03
1998	296	1300	763	977	57.4	18.3
1998	296	1305	757	974	56.77	18.25
1998	296	1310	753	974	56.47	18.4
1998	296	1315	748	974	56.34	18.56
1998	296	1320	742	973	56.25	18.6
1998	296	1325	738	973	55.54	18.81
1998	296	1330	730	972	56.03	18.95
1998	296	1335	722	968	54.64	18.99
1998	296	1340	714	964	53.62	18.84
1998	296	1345	704	962	54.8	18.95
1998	296	1350	693.3	958	54.34	19.14
1998	296	1355	687.2	961	52.78	19.05
1998	296	1400	677	959	53.87	19.25
1998	296	1405	665.6	956	54.5	19.56
1998	296	1410	653.4	951	53.87	19.51
1998	296	1415	641.4	946	53.04	19.41
1998	296	1420	628.9	943	53.04	19.4
1998	296	1425	616	936	51.87	19.67
1998	296	1430	604.1	932	51.13	19.73
1998	296	1435	591.9	928	51.06	19.68
1998	296	1440	578	917	49.7	19.6
1998	296	1445	564.8	912	49.64	19.29
1998	296	1450	552.7	909	49.26	19.55
1998	296	1455	540.4	910	49.69	19.88
1998	296	1500	525.9	901	46.55	19.57
1998	296	1505	511.8	900	46.42	19.54

1998	296	1510	498.8	898	45.32	19.61
1998	296	1515	484.5	890	42.97	19.25
1998	296	1520	469.1	883	42.44	19.19
1998	296	1525	453.6	876	41.64	19.02
1998	296	1530	439.7	873	42.82	19.49
1998	296	1535	423.4	863	41.28	19.13
1998	296	1540	406.7	854	42.53	19.43
1998	296	1545	390.8	843	41.86	19.56
1998	296	1550	375.3	835	39.92	19.39
1998	296	1555	359.1	827	39.54	19.45
1998	296	1600	343	818	36.45	19.2
1998	296	1605	324.6	808	35.25	19.02
1998	296	1610	303.9	796	35.33	19.12
1998	296	1615	284.5	783	34.3	19.23
1998	296	1620	266	767	32.06	19
1998	296	1625	248.6	753	30.63	18.84
1998	296	1630	231.1	741	30.36	18.9
1998	296	1635	213.1	723	28.99	18.87
1998	296	1640	194.9	702	26.87	18.62
1998	296	1645	176.9	680.8	25.65	18.54
1998	296	1650	159.5	660.4	24.31	18.47
1998	296	1655	142	638.4	23.66	18.67
1998	296	1700	123.9	610.6	22.42	18.8
1998	296	1705	106.4	579.2	19.76	18.63
1998	296	1710	89.8	545.6	17.12	18.43
1998	296	1715	73.4	512.3	15.66	18.46
1998	296	1720	57.03	469.3	14.09	18.64
1998	296	1725	41.86	422.2	11.52	18.67
1998	296	1730	27.63	369.4	9.16	18.71
1998	296	1735	14.55	308.1	5.396	18.41
1998	296	1740	3.703	233	1.676	17.99
1998	296	1745	-5.433	59.79	-0.556	17.81
1998	296	1750	-12.2	0.097	-3.02	17.63
1998	296	1755	-14.54	-1.13	-5.371	17.52
1998	296	1800	-15.99	-1.189	-6.972	17.43

24TH OCTOBER 1998

YEAR	DAY	TIME	GHI	DNI	DHI	TEMP
1998	297	1200	738	862	111.9	19.32
1998	297	1205	734	855	111	19.68
1998	297	1210	735	858	108.9	19.58
1998	297	1215	734	856	109.6	19.71
1998	297	1220	730	842	114.8	19.58
1998	297	1225	743	865	113.3	19.83
1998	297	1230	746	877	105.5	20.09
1998	297	1235	733	869	102.3	20.55
1998	297	1240	740	878	97.9	20.19
1998	297	1245	740	881	96.3	20.28
1998	297	1250	715	852	100.1	20.73
1998	297	1255	721	863	99.5	20.98
1998	297	1300	723	872	97.3	20.92
1998	297	1305	723	874	99.7	21.2
1998	297	1310	683.1	809	108.3	21.03
1998	297	1315	672.5	783	119.2	20.84
1998	297	1320	705	850	110.1	20.86
1998	297	1325	698.4	856	100.7	20.96
1998	297	1330	684.8	844	99.3	21.18
1998	297	1335	677.4	842	97.2	21.07
1998	297	1340	664.6	834	98.4	21.37
1998	297	1345	650.3	823	99.3	21.51
1998	297	1350	648.5	828	98.1	21.43
1998	297	1355	635.7	819	100.2	21.48
1998	297	1400	630.6	821	99.4	21.61
1998	297	1405	628.3	830	98.8	21.85
1998	297	1410	614.4	823	97.4	21.99
1998	297	1415	601.8	819	96	22.09
1998	297	1420	583.8	805	98.1	22.53
1998	297	1425	578.2	811	94.6	22.52
1998	297	1430	567.1	806	91.3	22.34
1998	297	1435	552.3	795	90.9	22.27
1998	297	1440	543.8	800	87.8	22.57
1998	297	1445	526	789	83.9	22.44
1998	297	1450	516.8	787	82.4	22.19
1998	297	1455	502.6	779	82.6	22.12
1998	297	1500	490	771	83.7	22.32
1998	297	1505	474.2	759	83.9	22.44
1998	297	1510	452.8	739	86.4	22.7
1998	297	1515	442.3	738	86.7	22.95
1998	297	1520	431.3	736	83.7	22.65
1998	297	1525	416.6	720	87.2	22.89
1998	297	1530	402.2	679.4	101	23.07
1998	297	1535	391.1	630.3	121.7	23.21
1998	297	1540	326.7	505.8	115.1	22.8
1998	297	1545	349.7	602.8	103.8	22.6

1998	297	1550	268.9	448.7	94.8	22.64
1998	297	1555	295.5	562.7	83.2	22.8
1998	297	1600	303.3	606	81.8	22.73
1998	297	1605	246	460.8	90.2	22.74
1998	297	1610	250.3	474	98.1	22.89
1998	297	1615	273.2	571.2	95.1	22.76
1998	297	1620	255	553.4	91.6	22.72
1998	297	1625	237.3	521.8	93.1	22.64
1998	297	1630	216.4	529.2	77.9	22.59
1998	297	1635	185.2	482.5	66.92	22.6
1998	297	1640	170.7	461.7	65.2	22.56
1998	297	1645	156.5	439.7	63.1	22.49
1998	297	1650	142.2	420.8	60.72	22.49
1998	297	1655	124.6	394.5	56.65	22.64
1998	297	1700	108.6	372	51.43	22.8
1998	297	1705	88	308.5	46.86	22.7
1998	297	1710	75.6	290.7	42.8	22.75
1998	297	1715	62.75	250.8	41.15	22.83
1998	297	1720	49.93	206.8	36.86	22.76
1998	297	1725	31.89	165.5	25.97	22.67
1998	297	1730	16.7	123.8	16.43	22.55
1998	297	1735	7.8	88.4	11.81	22.36
1998	297	1740	-0.37	51.39	6.356	22.29
1998	297	1745	-6.714	2.609	1.487	22.19
1998	297	1750	-11.18	-1.504	-2.037	22.08
1998	297	1755	-13.74	-2.46	-5	21.99
1998	297	1800	-15.13	-3.138	-7.06	21.88

29TH OCTOBER 1998

YEAR	DAY	TIME	GHI	DNI	DHI	TEMP
1998	302	1200	710	815	118.2	25.9
1998	302	1205	531.2	509.3	161.1	25.85
1998	302	1210	280.3	90.9	223.7	25.82
1998	302	1215	777	760	223.2	25.9
1998	302	1220	608.8	570.8	194.7	26.08
1998	302	1225	659.3	644.3	195.1	26.37
1998	302	1230	238.4	15.39	239.5	26.42
1998	302	1235	267.7	27.12	256.1	26.21
1998	302	1240	247.2	39.38	221.9	25.84
1998	302	1245	346.4	124.5	256	25.7
1998	302	1250	798	786	227.7	25.67
1998	302	1255	737	759	189.9	25.89
1998	302	1300	643.1	654.1	178.8	26.2
1998	302	1305	536	392.6	263.1	26.41
1998	302	1310	786	831	201.7	26.48
1998	302	1315	757	816	186.3	26.56
1998	302	1320	731	814	164.4	26.6
1998	302	1325	704	813	140.7	26.41
1998	302	1330	696.3	813	140.6	26.78
1998	302	1335	682	815	127.6	26.4
1998	302	1340	671.2	782	145.6	26.6
1998	302	1345	692.9	794	163.3	26.4
1998	302	1350	667.4	803	139.2	26.22
1998	302	1355	644.5	794	127.7	26.12
1998	302	1400	620.5	789	113.4	26.41
1998	302	1405	519.6	619.2	126.6	26.57
1998	302	1410	627.5	771	144.5	26.56
1998	302	1415	320.1	256.2	166.6	26.59
1998	302	1420	300	199.6	185.7	26.41
1998	302	1425	184.4	-2.956	195.7	25.93
1998	302	1430	212.8	39.36	197.7	25.79
1998	302	1435	328	203.6	215.5	25.97
1998	302	1440	180.4	0.194	191.4	26.21
1998	302	1445	161.5	-1.259	172.7	26.2
1998	302	1450	223.8	110.2	171.9	26.2
1998	302	1455	408.9	385.9	208.5	26.4
1998	302	1500	543.5	725	169.4	26.68
1998	302	1505	317.1	328.9	155	26.9
1998	302	1510	257.4	113.8	208.3	26.77
1998	302	1515	271.2	215.4	175.2	26.62
1998	302	1520	457.1	710	126.5	26.77
1998	302	1525	165.6	133.1	112.1	26.96
1998	302	1530	375.6	560.9	130.4	26.97
1998	302	1535	435.1	690.9	139.7	26.96
1998	302	1540	418.3	686	135.7	27.07
1998	302	1545	311	535.1	98.3	27.15

1998	302	1550	132.4	169.7	72.6	27
1998	302	1555	177.1	273.9	78.9	26.82
1998	302	1600	191.6	334.1	76.5	26.78
1998	302	1605	281.2	599	79.6	26.83
1998	302	1610	258.8	609.7	65.66	26.99
1998	302	1615	240.9	589.9	63.92	27.05
1998	302	1620	231.2	570.9	69.61	27.11
1998	302	1625	186.3	441.8	70.9	27.27
1998	302	1630	57.8	38.29	58.07	27.24
1998	302	1635	59.58	80.1	48.22	27.08
1998	302	1640	69.5	105	52.41	26.93
1998	302	1645	84.7	170.7	55.65	26.81
1998	302	1650	88	221.1	50.76	26.64
1998	302	1655	98.6	342.9	41.36	26.45
1998	302	1700	85.7	329.7	37.03	26.42
1998	302	1705	70.1	282.9	34.06	26.43
1998	302	1710	54.56	229.9	31.42	26.5
1998	302	1715	43.56	214.8	26.08	26.61
1998	302	1720	26.93	128.7	20.79	26.62
1998	302	1725	13.57	71.7	15.33	26.45
1998	302	1730	5.854	73.7	7.55	26.27
1998	302	1735	-2.655	22.78	1.449	26.1
1998	302	1740	-8.43	-2.001	-2.855	25.97
1998	302	1745	-11.14	-2.453	-5.785	25.84
1998	302	1750	-12.88	-2.814	-7.83	25.78
1998	302	1755	-14.13	-2.698	-8.85	25.72
1998	302	1800	-14.56	-2.421	-9.45	25.65

6TH APRIL
1999

YEAR	DAY	TIME	GHI	DNI	DHI	TEMP
1999	96	1200	968	953	101.3	25.01
1999	96	1205	976	959	99.4	24.85
1999	96	1210	986	968	98.8	24.97
1999	96	1215	984	968	96.8	25.3
1999	96	1220	980	969	93.5	25.77
1999	96	1225	981	965	95.3	25.78
1999	96	1230	985	956	103.6	25.58
1999	96	1235	986	952	107.8	25.66
1999	96	1240	987	952	113.6	26.53
1999	96	1245	986	932	129.9	26.81
1999	96	1250	985	935	128.6	27.09
1999	96	1255	971	927	117.1	26.5
1999	96	1300	962	925	114.2	26.95
1999	96	1305	957	924	110.1	26.91
1999	96	1310	949	915	111.7	26.81
1999	96	1315	949	920	113	27.24
1999	96	1320	949	923	111.3	27.29
1999	96	1325	945	922	114.5	27.22
1999	96	1330	941	918	118.6	27.33
1999	96	1335	944	917	126.5	27.5
1999	96	1340	941	908	133.6	27.34
1999	96	1345	942	908	141	27.36
1999	96	1350	934	901	141.9	26.98
1999	96	1355	930	902	146.9	27.72
1999	96	1400	911	870	158.5	27.68
1999	96	1405	909	847	180	27.25
1999	96	1410	788	687.4	201	27.26
1999	96	1415	855	780	196.8	27.21
1999	96	1420	768	727	158.8	27.29
1999	96	1425	841	843	144	27.12
1999	96	1430	850	860	147.8	27.37
1999	96	1435	835	859	142.3	27.72
1999	96	1440	812	824	155.5	27.72
1999	96	1445	744	682.2	204	27.42
1999	96	1450	438.3	254.5	239.3	27.23
1999	96	1455	377.2	147.2	267.9	27.26
1999	96	1500	770	647.6	283.2	27.42
1999	96	1505	647.4	545.3	240.4	27.33
1999	96	1510	511.8	371.7	241	27.57
1999	96	1515	525.3	405.9	235.1	27.49
1999	96	1520	798	834	211.3	27.68
1999	96	1525	633.1	666.3	170.5	27.71
1999	96	1530	576.5	601.2	167.8	27.78
1999	96	1535	604.5	641.3	175.8	27.68
1999	96	1540	495.1	461.2	192.4	27.41

1999	96	1545	353.9	223.4	213.4	27.5
1999	96	1550	524.1	442.9	253	27.7
1999	96	1555	650.5	693	230	27.82
1999	96	1600	497.6	523.2	188.9	27.68
1999	96	1605	417.1	389.7	195.3	27.95
1999	96	1610	432.7	416.7	200.5	27.78
1999	96	1615	260.6	151.5	183.1	27.69
1999	96	1620	190.7	32.78	181.8	27.46
1999	96	1625	209.1	33.18	197.7	27.17
1999	96	1630	202.6	16.68	200.8	27.05
1999	96	1635	263.9	99.7	222	27.18
1999	96	1640	199.3	12.26	202.7	27.26
1999	96	1645	167.4	0.239	175.2	27.07
1999	96	1650	158.4	-0.639	166.2	26.92
1999	96	1655	148.8	-1.329	156.8	26.87
1999	96	1700	147	-0.303	153.2	26.74
1999	96	1705	217.5	142.8	165.7	26.67
1999	96	1710	213.9	95	182.2	26.66
1999	96	1715	272.1	250.2	186.6	26.67
1999	96	1720	219.1	175.2	163.7	26.64
1999	96	1725	188.9	176.9	137.4	26.63
1999	96	1730	255.5	399.7	139.9	26.7
1999	96	1735	173.6	172.9	129.7	26.63
1999	96	1740	125.9	95.4	106	26.56
1999	96	1745	73.5	0.491	80.7	26.42
1999	96	1750	62.94	2.317	68.46	26.22
1999	96	1755	55.34	11.87	57.7	26.03
1999	96	1800	51.68	-2.033	57.28	25.82

Appendix B

Mass Spectrometry Data

Information from Data File:
File: C:\SARAH\SC1-1.D
Operator:
Date Acquired: 2 Nov 1998 12:35 pm
Method File: TO15D
Sample Name: smog chamber 2:25-2:27 pm 10-23-98
Misc Info:
Vial Number: 1

Search Libraries: C:\DATABASE\NBS75K.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - VOCS.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	0.14	0.05	C:\DATABASE\NBS75K.L			
			Acetic acid, oxo-	305	000298-12-4	3
			Ethane	62248	000074-84-0	2
			Ethane	62247	000074-84-0	2
2	2.70	20.45	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	4
			Ethylene oxide	62266	000075-21-8	4
			Acetaldehyde	36	000075-07-0	3
3	2.94	55.30	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	4
			Ethylene oxide	62266	000075-21-8	4
			Acetaldehyde	62265	000075-07-0	3
4	3.37	3.63	C:\DATABASE\NBS75K.L			
			Dichlorotetrafluoroethane	14961	000076-14-2	58
			Dichlorotetrafluoroethane	68163	000076-14-2	58
			Dichlorodifluoromethane	64510	000075-71-8	22
5	3.61	0.15	C:\DATABASE\NBS75K.L			
			1,3-Cyclohexanediol	3291	000504-01-8	9
			Piperazine	62810	000110-85-0	9
			2-Propenal	72	000107-02-8	4
6	3.72	0.15	C:\DATABASE\NBS75K.L			
			Butane	62336	000106-97-8	9
			Butane	99	000106-97-8	9
			Acetaldehyde	62264	000075-07-0	7
7	3.86	0.17	C:\DATABASE\NBS75K.L			
			Benzenemethanol, .alpha.-(1-aminoe	66861	014838-15-4	9
			Propane	62269	000074-98-6	4
			Amphetamine	65612	000300-62-9	4
8	4.09	0.12	C:\DATABASE\NBS75K.L			
			Benzenemethanol, .alpha.-(1-aminoe	66861	014838-15-4	9
			Ethylene oxide	62266	000075-21-8	4
			Propane	62269	000074-98-6	4
9	4.75	0.20	C:\DATABASE\NBS75K.L			
			Cyclopropane, 1,2-dimethyl-, cis-	62467	000930-18-7	53
			1-Butene, 2-methyl-	62457	000563-46-2	46
			1-Butene, 3-methyl-	236	000563-45-1	46
10	5.28	0.33	C:\DATABASE\NBS75K.L			
			Butane, 2-methyl-	62518	000078-78-4	64
			Butane, 2-methyl-	62517	000078-78-4	64
			Butane, 2-methyl-	281	000078-78-4	42
11	5.42	0.15	C:\DATABASE\NBS75K.L			
			2-Octanamine, N-(1-methylheptyl)-	71215	005412-92-0	40
			Acetone	62325	000067-64-1	17
			2-Propanamine	62339	000075-31-0	9

12 5.84 0.18 C:\DATABASE\NBS75K.L
1-Pentene 230 000109-67-1 58
1-Pentene 62466 000109-67-1 58
Cyclopropane, ethyl- 227 001191-96-4 49

13 6.37 0.15 C:\DATABASE\NBS75K.L
Pentane 280 000109-66-0 38
Butane, 2-methyl- 62518 000078-78-4 16
Butane, 2-methyl- 62517 000078-78-4 16

14 6.63 0.14 C:\DATABASE\NBS75K.L
1,3-Butadiene, 2-methyl- 62410 000078-79-5 91
1,3-Butadiene, 2-methyl- 184 000078-79-5 83
1,3-Butadiene, 2-methyl- 62408 000078-79-5 81

15 6.86 0.16 C:\DATABASE\NBS75K.L
Cyclopropane, 1,2-dimethyl-, cis- 62467 000930-18-7 58
2-Pentene, (Z)- 62456 000627-20-3 53
1-Butene, 3-methyl- 236 000563-45-1 53

16 7.35 0.16 C:\DATABASE\NBS75K.L
2-Butene, 2-methyl- 62461 000513-35-9 58
2-Pentene, (Z)- 62456 000627-20-3 53
1-Butene, 2-methyl- 62457 000563-46-2 52

17 7.66 0.16 C:\DATABASE\NBS75K.L
Cyclopropane, 1,2-dimethyl-, cis- 62467 000930-18-7 68
2-Butene, 2-methyl- 62461 000513-35-9 68
Cyclopropane, 1,2-dimethyl-, trans 62459 002402-06-4 59

18 8.53 0.27 C:\DATABASE\NBS75K.L
Butane, 2,2-dimethyl- 732 000075-83-2 53
Butane, 2,2-dimethyl- 62861 000075-83-2 53
Butane, 2,2-dimethyl- 62862 000075-83-2 53

19 9.45 0.21 C:\DATABASE\NBS75K.L
Cyclopentene 185 000142-29-0 81
Cyclopentene 62412 000142-29-0 80
Cyclopentene 62411 000142-29-0 72

20 9.76 0.24 C:\DATABASE\NBS75K.L
1-Butanol 62581 000071-36-3 53
1-Pentene, 4-methyl- 599 000691-37-2 52
2-Butene, (E)- 62302 000624-64-6 47

21 10.02 0.19 C:\DATABASE\NBS75K.L
1-Pentene 62465 000109-67-1 81
1-Pentene 62464 000109-67-1 59
Cyclopentane 234 000287-92-3 59

22 10.20 0.25 C:\DATABASE\NBS75K.L
Butane, 2,3-dimethyl- 62870 000079-29-8 80
Butane, 2,3-dimethyl- 62871 000079-29-8 80
Butane, 2,3-dimethyl- 62869 000079-29-8 72

23 10.47 0.28 C:\DATABASE\NBS75K.L
Pentane, 2-methyl- 733 000107-83-5 87
Pentane, 2-methyl- 62865 000107-83-5 80
Pentane, 2-methyl- 62863 000107-83-5 80

24 10.78 0.05 C:\DATABASE\NBS75K.L
Butanal 62487 000123-72-8 58
Butanal 265 000123-72-8 53
Butanal 62486 000123-72-8 53

25 11.17 0.29 C:\DATABASE\NBS75K.L
Pentane, 3-methyl- 62868 000096-14-0 72
Pentane, 3-methyl- 62867 000096-14-0 72
Pentane, 3-methyl- 734 000096-14-0 46

26 11.44 0.22 C:\DATABASE\NBS75K.L
Cyclohexane 62779 000110-82-7 74
1-Pentene, 2-methyl- 62768 000763-29-1 68
Cyclohexane 606 000110-82-7 64

27 12.05 0.31 C:\DATABASE\NBS75K.L
Hexane 62874 000110-54-3 80
Hexane 62873 000110-54-3 59
Hexane 736 000110-54-3 58

28 12.28 0.25 C:\DATABASE\NBS75K.L
2-Hexene 589 000592-43-8 87
2-Hexene, (E)- 62752 004050-45-7 83
2-Hexene, (E)- 62751 004050-45-7 83

29 12.67 0.25 C:\DATABASE\NBS75K.L
2-Hexene, (E)- 62751 004050-45-7 93
2-Hexene 589 000592-43-8 87
2-Hexene, (E)- 62752 004050-45-7 83

30 13.14 0.27 C:\DATABASE\NBS75K.L
Cyclopentane, methyl- 594 000096-37-7 87
Cyclopentane, methyl- 62763 000096-37-7 74
Cyclohexane 62777 000110-82-7 72

31 13.37 0.35 C:\DATABASE\NBS75K.L
Pentane, 2,4-dimethyl- 1594 000108-08-7 87
Pentane, 2,4-dimethyl- 63424 000108-08-7 83
Pentane, 2,4-dimethyl- 63425 000108-08-7 80

32 14.13 0.32 C:\DATABASE\NBS75K.L
Benzene 62628 000071-43-2 94
Benzene 62627 000071-43-2 91
Benzene 62626 000071-43-2 91

33 14.48 0.40 C:\DATABASE\NBS75K.L
Cyclohexane 62777 000110-82-7 93
Cyclohexane 606 000110-82-7 87
Cyclohexane 62776 000110-82-7 87

34 14.85 0.52 C:\DATABASE\NBS75K.L
Hexane, 2-methyl- 63435 000591-76-4 90
Hexane, 2-methyl- 63433 000591-76-4 86
Hexane, 2-methyl- 1598 000591-76-4 80

35 14.91 0.47 C:\DATABASE\NBS75K.L
Pentane, 2,3-dimethyl- 63429 000565-59-3 91
Pentane, 2,3-dimethyl- 63432 000565-59-3 78
Pentane, 2,3-dimethyl- 63431 000565-59-3 70

36 15.17 0.51 C:\DATABASE\NBS75K.L
Hexane, 3-methyl- 63422 000589-34-4 81
Hexane, 3-methyl- 1593 000589-34-4 72
Hexane, 3-methyl- 63423 000589-34-4 68

37 15.64 0.68 C:\DATABASE\NBS75K.L
Heptane, 2,2,4,6,6-pentamethyl- 68260 013475-82-6 78
Pentane, 2,2,4-trimethyl- 64220 000540-84-1 72
Pentane, 2,2,4,4-tetramethyl- 65105 001070-87-7 64

38 15.91 1.75 C:\DATABASE\NBS75K.L
Benzene, methyl-, trifluoro deriv. 8769 027359-10-0 96
Benzene, (trifluoromethyl)- 66428 000098-08-8 94
Benzene, (trifluoromethyl)- 8768 000098-08-8 93

39 16.01 0.47 C:\DATABASE\NBS75K.L
Heptane 63438 000142-82-5 91
Heptane 63440 000142-82-5 90
Heptane 1600 000142-82-5 86

40 16.70 0.50 C:\DATABASE\NBS75K.L

Cyclohexane, methyl- 1326 000108-87-2 96
Cyclohexane, methyl- 63236 000108-87-2 96
Cyclohexane, methyl- 63235 000108-87-2 94

41 17.62 0.62 C:\DATABASE\NBS75K.L
Pentane, 2,3,4-trimethyl- 3100 000565-75-3 91
Pentane, 2,3,4-trimethyl- 64228 000565-75-3 86
Pentane, 2,3,4-trimethyl- 64229 000565-75-3 78

42 17.76 0.43 C:\DATABASE\NBS75K.L
Toluene 63028 000108-88-3 95
Toluene 965 000108-88-3 93
Toluene 63029 000108-88-3 90

43 18.06 0.67 C:\DATABASE\NBS75K.L
Heptane, 2-methyl- 3092 000592-27-8 91
Heptane, 2-methyl- 64218 000592-27-8 87
Hexane, 2,5-dimethyl- 64206 000592-13-2 64

44 18.28 0.63 C:\DATABASE\NBS75K.L
Heptane, 3-methyl- 64227 000589-81-1 64
Pentane, 2,4-dimethyl- 1594 000108-08-7 59
Heptane, 3-methyl- 3099 000589-81-1 58

45 18.99 0.63 C:\DATABASE\NBS75K.L
Octane 3084 000111-65-9 87
Octane 64207 000111-65-9 81
Hexane, 2,4-dimethyl- 64212 000589-43-5 59

46 20.40 0.50 C:\DATABASE\NBS75K.L
Ethylbenzene 2026 000100-41-4 93
Ethylbenzene 63690 000100-41-4 93
Ethylbenzene 63692 000100-41-4 93

47 20.64 0.93 C:\DATABASE\NBS75K.L
p-Xylene 63702 000106-42-3 95
p-Xylene 63699 000106-42-3 94
Benzene, 1,2-dimethyl- 63707 000095-47-6 94

48 21.12 0.29 C:\DATABASE\NBS75K.L
Styrene 63645 000100-42-5 95
Styrene 63646 000100-42-5 94
1,3,5,7-Cyclooctatetraene 1949 000629-20-9 94

49 21.27 0.47 C:\DATABASE\NBS75K.L
Benzene, 1,3-dimethyl- 63695 000108-38-3 95
Benzene, 1,2-dimethyl- 63706 000095-47-6 94
Benzene, 1,2-dimethyl- 63705 000095-47-6 94

50 21.63 0.73 C:\DATABASE\NBS75K.L
Nonane 65142 000111-84-2 90
Nonane 5163 000111-84-2 58
Octane 64207 000111-65-9 50

51 21.92 0.32 C:\DATABASE\NBS75K.L
Benzene, 1-bromo-3-fluoro- 16034 001073-06-9 97
Benzene, 1-bromo-2-fluoro- 16035 001072-85-1 93
Benzene, 1-bromo-2-fluoro- 68408 001072-85-1 93

52 22.15 0.56 C:\DATABASE\NBS75K.L
Benzene, (1-methylethyl)- 64555 000098-82-8 95
Benzene, (1-methylethyl)- 3763 000098-82-8 95
Benzene, (1-methylethyl)- 64556 000098-82-8 94

53 22.69 0.09 C:\DATABASE\NBS75K.L
Benzaldehyde 63689 000100-52-7 96
Benzaldehyde 63685 000100-52-7 95
Benzaldehyde 63686 000100-52-7 90

54 22.75 0.14 C:\DATABASE\NBS75K.L
.alpha.-Pinene 65808 000080-56-8 93

.alpha.-Pinene 65809 000080-56-8 90
Tricyclo[2.2.1.02,6]heptane, 1,7,7 6668 000508-32-7 81

55 22.97 0.55 C:\DATABASE\NBS75K.L
Benzene, propyl- 64583 000103-65-1 91
Benzene, propyl- 3781 000103-65-1 90
Benzene, propyl- 64582 000103-65-1 90

56 23.19 0.19 C:\DATABASE\NBS75K.L
Camphene 65764 000079-92-5 97
Camphene 65765 000079-92-5 95
Camphene 65767 000079-92-5 95

57 23.36 0.45 C:\DATABASE\NBS75K.L
Benzene, 1,3,5-trimethyl- 64570 000108-67-8 97
1,2,4-Trimethylbenzene 3771 000095-36-3 96
Benzene, 1,2,3-trimethyl- 64572 000526-73-8 95

58 24.12 0.52 C:\DATABASE\NBS75K.L
Benzene, 1,2,3-trimethyl- 64572 000526-73-8 95
Benzene, 1,2,4-trimethyl- 64578 000095-63-6 95
Benzene, 1,2,3-trimethyl- 64573 000526-73-8 95

59 25.00 0.11 C:\DATABASE\NBS75K.L
Benzene, 1-methyl-2-(1-methylethyl 65581 000527-84-4 95
Benzene, 1-methyl-2-(1-methylethyl 6228 000527-84-4 94
Benzene, 1-methyl-4-(1-methylethyl 65534 000099-87-6 94

60 25.31 0.12 C:\DATABASE\NBS75K.L
Limonene 65777 000138-86-3 95
D-Limonene 6664 005989-27-5 95
D-Limonene 65790 005989-27-5 94

61 25.75 0.07 C:\DATABASE\NBS75K.L
Acetophenone 64533 000098-86-2 94
Acetophenone 64537 000098-86-2 93
Acetophenone 64535 000098-86-2 70

62 25.93 0.06 C:\DATABASE\NBS75K.L
Ethane, 1,1,2-trichloro-1,2,2-trif 69052 000076-13-1 53
Ethane, 1,1,2-trichloro-1,2,2-trif 69050 000076-13-1 47
Methane, bromodichlorofluoro- 17512 000353-58-2 38

63 26.85 0.05 C:\DATABASE\NBS75K.L
Benzene, 1-methyl-4-(1-methylethen 65410 001195-32-0 96
o-Isopropenyltoluene 5877 007399-49-7 95
Benzene, methyl(1-methylethenyl)- 5892 026444-18-8 95

64 27.37 0.15 C:\DATABASE\NBS75K.L
Butane, 1,1,3,4-tetrachloro-1,2,2, 42990 000423-38-1 64
Pentane, 1,1,2,3,4,5-hexachloro-1, 52447 055975-93-4 43
Ethane, 1,1,2-trichloro-1,2,2-trif 69052 000076-13-1 40

Sun Jun 27 16:47:30 1999

Information from Data File:
File: C:\SARAH\SC1-2.D
Operator:
Date Acquired: 2 Nov 1998 4:56 pm
Method File: TO15D
Sample Name: smog chamber 615 10-23-98
Misc Info:
Vial Number: 1

Search Libraries: C:\DATABASE\NBS75K.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - VOCS.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	0.16	0.03	C:\DATABASE\NBS75K.L			
			Acetic acid, oxo-	305	000298-12-4	3
			Ethane	62248	000074-84-0	2
			Ethane	62247	000074-84-0	2
2	0.26	0.09	C:\DATABASE\NBS75K.L			
			Piperidine, 1-nitro-	5328	007119-94-0	4
			Acetic acid, oxo-	305	000298-12-4	3
			Ethane	62248	000074-84-0	2
3	0.32	0.13	C:\DATABASE\NBS75K.L			
			Piperidine, 1-nitro-	5328	007119-94-0	4
			Ethane	62248	000074-84-0	2
			Ethane	62247	000074-84-0	2
4	0.56	0.03	C:\DATABASE\NBS75K.L			
			Piperidine, 1-nitro-	5328	007119-94-0	4
			Acetic acid, oxo-	305	000298-12-4	2
			Ethane	62247	000074-84-0	2
5	2.70	19.90	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	4
			Ethylene oxide	62266	000075-21-8	4
			Acetaldehyde	62264	000075-07-0	3
6	2.83	13.36	C:\DATABASE\NBS75K.L			
			Carbon dioxide	34	000124-38-9	3
			Ethylene oxide	62267	000075-21-8	3
			Carbon dioxide	62263	000124-38-9	3
7	2.95	52.39	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	4
			Ethylene oxide	62266	000075-21-8	4
			Acetaldehyde	62265	000075-07-0	3
8	3.37	3.47	C:\DATABASE\NBS75K.L			
			Dichlorotetrafluoroethane	68163	000076-14-2	62
			Dichlorotetrafluoroethane	14961	000076-14-2	58
			Dichlorodifluoromethane	64510	000075-71-8	27
9	3.61	0.06	C:\DATABASE\NBS75K.L			
			Carbon dioxide	62263	000124-38-9	4
			Carbon dioxide	34	000124-38-9	4
			Acetaldehyde	36	000075-07-0	4
10	3.72	0.15	C:\DATABASE\NBS75K.L			
			Carbon dioxide	34	000124-38-9	4
			Carbon dioxide	62263	000124-38-9	4
			Amphetamine	65612	000300-62-9	4
11	4.76	0.07	C:\DATABASE\NBS75K.L			
			Cyclopropane, 1,1-dimethyl-	235	001630-94-0	10
			2-Butene, 2-methyl-	62462	000513-35-9	10
			Cyclopropane, 1,2-dimethyl-, cis-	62467	000930-18-7	10

12 5.28 0.22 C:\DATABASE\NBS75K.L
Butane, 2-methyl- 62518 000078-78-4 52
Butane, 2-methyl- 62517 000078-78-4 52
Oxirane, 2,2-dimethyl- 62511 000558-30-5 35

13 5.47 0.23 C:\DATABASE\NBS75K.L
Acetone 62323 000067-64-1 38
Acetone 62325 000067-64-1 38
Acetone 62324 000067-64-1 38

14 5.57 0.21 C:\DATABASE\NBS75K.L
Acetone 62326 000067-64-1 58
Acetone 62324 000067-64-1 53
Acetone 62325 000067-64-1 53

15 5.84 0.03 C:\DATABASE\NBS75K.L
Ethylene oxide 62267 000075-21-8 4
n-Hexylmethylamine 3165 035161-70-7 4
2-Heptanamine, 5-methyl- 65167 053907-81-6 4

16 6.38 0.11 C:\DATABASE\NBS75K.L
Pentane 280 000109-66-0 50
Butane, 2-methyl- 62517 000078-78-4 37
1,4-Butanediol 62986 000110-63-4 33

17 8.53 0.18 C:\DATABASE\NBS75K.L
Butane, 2,2-dimethyl- 62861 000075-83-2 80
Butane, 2,2-dimethyl- 732 000075-83-2 72
Butane, 2,2-dimethyl- 62862 000075-83-2 72

18 9.76 0.07 C:\DATABASE\NBS75K.L
(E)-1-Hydroxy-1,3-butadiene 207 000000-00-0 47
1-Propene, 2-methyl- 62305 000115-11-7 46
1-Propene, 2-methyl- 78 000115-11-7 38

19 10.02 0.11 C:\DATABASE\NBS75K.L
Cyclopentane 234 000287-92-3 72
1-Pentene 62464 000109-67-1 72
1-Pentene 62466 000109-67-1 64

20 10.20 0.16 C:\DATABASE\NBS75K.L
Butane, 2,3-dimethyl- 62870 000079-29-8 86
Butane, 2,3-dimethyl- 62871 000079-29-8 72
Butane, 2,3-dimethyl- 62869 000079-29-8 64

21 10.47 0.16 C:\DATABASE\NBS75K.L
Pentane, 2-methyl- 62863 000107-83-5 80
Pentane, 2-methyl- 62865 000107-83-5 80
Pentane, 2-methyl- 733 000107-83-5 74

22 10.57 0.03 C:\DATABASE\NBS75K.L
2-Pentene, (Z)- 62456 000627-20-3 38
1-Butene, 3-methyl- 236 000563-45-1 38
2-Pentene 231 000109-68-2 38

23 10.80 0.07 C:\DATABASE\NBS75K.L
Butanal 62487 000123-72-8 90
Butanal 62489 000123-72-8 90
Butanal 62488 000123-72-8 83

24 11.16 0.24 C:\DATABASE\NBS75K.L
Pentane, 3-methyl- 734 000096-14-0 72
Pentane, 3-methyl- 62867 000096-14-0 72
Hexane, 3,4-dimethyl- 3086 000583-48-2 42

25 12.03 0.16 C:\DATABASE\NBS75K.L
Hexane 62874 000110-54-3 80
Hexane 62872 000110-54-3 52
Hexane 736 000110-54-3 52

26 13.14 0.15 C:\DATABASE\NBS75K.L
Cyclopentane, methyl- 594 000096-37-7 87
Cyclopentane, methyl- 62763 000096-37-7 64
Cyclobutane, ethyl- 604 004806-61-5 64

27 13.38 0.29 C:\DATABASE\NBS75K.L
Pentane, 2,4-dimethyl- 63425 000108-08-7 80
Pentane, 2,4-dimethyl- 1594 000108-08-7 58
Butane, 2,2,3-trimethyl- 1599 000464-06-2 50

28 14.14 0.24 C:\DATABASE\NBS75K.L
Benzene 62628 000071-43-2 91
Benzene 62627 000071-43-2 91
Benzene 62626 000071-43-2 91

29 14.48 0.22 C:\DATABASE\NBS75K.L
Cyclohexane 62777 000110-82-7 93
Cyclohexane 606 000110-82-7 87
Cyclohexane 62776 000110-82-7 87

30 14.87 0.30 C:\DATABASE\NBS75K.L
Hexane, 2-methyl- 63435 000591-76-4 87
Hexane, 2-methyl- 1598 000591-76-4 87
Hexane, 2-methyl- 63433 000591-76-4 80

31 14.93 0.36 C:\DATABASE\NBS75K.L
Pentane, 2,3-dimethyl- 63432 000565-59-3 53
Pentane, 2,3-dimethyl- 63429 000565-59-3 45
Pentane, 2,3-dimethyl- 63431 000565-59-3 45

32 15.18 0.29 C:\DATABASE\NBS75K.L
Hexane, 3-methyl- 1593 000589-34-4 72
Hexane, 3-methyl- 63421 000589-34-4 68
Hexane, 3-methyl- 63422 000589-34-4 58

33 15.65 0.44 C:\DATABASE\NBS75K.L
Heptane, 2,2,4,6,6-pentamethyl- 68260 013475-82-6 78
Hexane, 2,2-dimethyl- 64216 000590-73-8 72
Pentane, 2,2,4-trimethyl- 64220 000540-84-1 72

34 15.92 1.39 C:\DATABASE\NBS75K.L
Benzene, methyl-, trifluoro deriv. 8769 027359-10-0 96
Benzene, (trifluoromethyl)- 66428 000098-08-8 94
Benzene, (trifluoromethyl)- 8768 000098-08-8 93

35 16.02 0.25 C:\DATABASE\NBS75K.L
Heptane 63438 000142-82-5 93
Heptane 63439 000142-82-5 87
Heptane 63440 000142-82-5 87

36 16.37 0.12 C:\DATABASE\NBS75K.L
1-Pentene, 2,4,4-trimethyl- 2693 000107-39-1 62
2-Hexene, 5,5-dimethyl-, (Z)- 64046 039761-61-0 52
1-Pentene, 2,4,4-trimethyl- 64024 000107-39-1 52

37 16.71 0.25 C:\DATABASE\NBS75K.L
Cyclohexane, methyl- 1326 000108-87-2 94
Cyclohexane, methyl- 63235 000108-87-2 87
Cyclohexane, methyl- 63236 000108-87-2 76

38 17.63 0.35 C:\DATABASE\NBS75K.L
Pentane, 2,3,4-trimethyl- 3100 000565-75-3 86
Pentane, 3-ethyl- 1595 000617-78-7 78
Pentane, 2,3,4-trimethyl- 64228 000565-75-3 78

39 17.77 0.27 C:\DATABASE\NBS75K.L
Toluene 63028 000108-88-3 93
Toluene 965 000108-88-3 93
Toluene 63029 000108-88-3 93

40 18.07 0.37 C:\DATABASE\NBS75K.L

Heptane, 2-methyl- 3092 000592-27-8 91
Hexane, 2,5-dimethyl- 64206 000592-13-2 86
Heptane, 2-methyl- 64218 000592-27-8 81

41 18.29 0.33 C:\DATABASE\NBS75K.L
Heptane, 3-methyl- 64227 000589-81-1 87
Heptane, 3-methyl- 3099 000589-81-1 72
Pentane, 2,4-dimethyl- 1594 000108-08-7 59

42 18.99 0.31 C:\DATABASE\NBS75K.L
Octane 64209 000111-65-9 90
Octane 3084 000111-65-9 87
Octane 64207 000111-65-9 87

43 20.41 0.29 C:\DATABASE\NBS75K.L
Ethylbenzene 63690 000100-41-4 93
Ethylbenzene 2026 000100-41-4 93
Ethylbenzene 63694 000100-41-4 93

44 20.66 0.37 C:\DATABASE\NBS75K.L
p-Xylene 63699 000106-42-3 95
Benzene, 1,3-dimethyl- 63695 000108-38-3 95
Benzene, 1,2-dimethyl- 63705 000095-47-6 94

45 21.28 0.22 C:\DATABASE\NBS75K.L
Benzene, 1,2-dimethyl- 63706 000095-47-6 93
Benzene, 1,3-dimethyl- 63697 000108-38-3 93
Benzene, 1,2-dimethyl- 63705 000095-47-6 93

46 21.64 0.32 C:\DATABASE\NBS75K.L
Nonane 65142 000111-84-2 87
Undecane 67317 001120-21-4 59
Nonane 65143 000111-84-2 49

47 21.93 0.24 C:\DATABASE\NBS75K.L
Benzene, 1-bromo-3-fluoro- 16034 001073-06-9 97
Benzene, 1-bromo-2-fluoro- 16035 001072-85-1 95
Benzene, 1-bromo-3-fluoro- 68407 001073-06-9 94

48 22.16 0.33 C:\DATABASE\NBS75K.L
Benzene, (1-methylethyl)- 3763 000098-82-8 94
Benzene, (1-methylethyl)- 64553 000098-82-8 93
Benzene, (1-methylethyl)- 64554 000098-82-8 93

49 22.70 0.06 C:\DATABASE\NBS75K.L
Benzaldehyde 63689 000100-52-7 96
Benzaldehyde 63688 000100-52-7 96
Benzaldehyde 63685 000100-52-7 89

50 22.98 0.29 C:\DATABASE\NBS75K.L
Benzene, propyl- 64584 000103-65-1 90
Benzene, propyl- 64582 000103-65-1 90
Benzene, propyl- 3781 000103-65-1 90

51 23.37 0.04 C:\DATABASE\NBS75K.L
1,2,4-Trimethylbenzene 3771 000095-36-3 87
Benzene, 1-ethyl-2-methyl- 64558 000611-14-3 86
Benzene, 1,2,4-trimethyl- 64578 000095-63-6 55

52 24.13 0.10 C:\DATABASE\NBS75K.L
Benzene, 1,3,5-trimethyl- 64571 000108-67-8 95
Benzene, 1,2,4-trimethyl- 64579 000095-63-6 94
Benzene, 1,2,3-trimethyl- 64573 000526-73-8 94

53 25.76 0.04 C:\DATABASE\NBS75K.L
Acetophenone 64538 000098-86-2 81
Acetophenone 64537 000098-86-2 74
Acetophenone 64536 000098-86-2 74

54 25.95 0.03 C:\DATABASE\NBS75K.L
Ethane, 1,1,2-trichloro-1,2,2-trif 69052 000076-13-1 50

Ethane, 1,1,2-trichloro-1,2,2-trif 69050 000076-13-1 40
Ethane, 1,1,2-trichloro-1,2,2-trif 69051 000076-13-1 40

55 27.39 0.07 C:\DATABASE\NBS75K.L
Butane, 1,2,3,4-tetrachloro-1,1,2, 42989 000375-45-1 38
Butane, 1,1,3,4-tetrachloro-1,2,2, 42990 000423-38-1 38
Butane, trichloroheptafluoro- 40359 028984-80-7 32

Sun Jun 27 16:54:01 1999

Information from Data File:
File: C:\SARAH\SC2-1.D
Operator:
Date Acquired: 2 Nov 1998 1:47 pm
Method File: TO15D
Sample Name: smog chamber 115 10-24-98
Misc Info:
Vial Number: 1

Search Libraries: C:\DATABASE\NBS75K.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - VOCS.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	0.25	0.04	C:\DATABASE\NBS75K.L			
			Piperidine, 1-nitro-	5328	007119-94-0	4
			2-Nitro-1-propanol	1961	002902-96-7	2
			Ethane	62248	000074-84-0	2
2	0.47	0.03	C:\DATABASE\NBS75K.L			
			Propane	62269	000074-98-6	3
			Propane	62268	000074-98-6	2
			Ethane	62248	000074-84-0	2
3	2.70	20.28	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	4
			Ethylene oxide	62266	000075-21-8	4
			Ethyne, fluoro-	35	002713-09-9	3
4	2.92	52.84	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	4
			Ethylene oxide	62266	000075-21-8	4
			Acetaldehyde	62265	000075-07-0	3
5	3.36	3.50	C:\DATABASE\NBS75K.L			
			Dichlorotetrafluoroethane	68163	000076-14-2	62
			Dichlorotetrafluoroethane	14961	000076-14-2	58
			Dichlorodifluoromethane	64510	000075-71-8	35
6	3.61	0.40	C:\DATABASE\NBS75K.L			
			2-Oxetanone, 4,4-dimethyl-	1450	001823-52-5	40
			1-Butene	62309	000106-98-9	20
			1-Butene	62308	000106-98-9	20
7	3.72	0.33	C:\DATABASE\NBS75K.L			
			Butane	62336	000106-97-8	25
			Butane	99	000106-97-8	14
			1-Propen-2-ol, acetate	1477	000108-22-5	10
8	3.86	0.32	C:\DATABASE\NBS75K.L			
			2-Oxetanone, 4,4-dimethyl-	1450	001823-52-5	53
			1-Propene, 2-methyl-	62305	000115-11-7	38
			1-Butene	62307	000106-98-9	38
9	4.09	0.14	C:\DATABASE\NBS75K.L			
			2-Oxetanone, 4,4-dimethyl-	1450	001823-52-5	53
			1-Butene	62307	000106-98-9	46
			1-Butene	62308	000106-98-9	41
10	4.76	0.21	C:\DATABASE\NBS75K.L			
			Cyclopropane, 1,2-dimethyl-, cis-	62467	000930-18-7	60
			1-Butene, 3-methyl-	236	000563-45-1	53
			1-Butene, 2-methyl-	62457	000563-46-2	49
11	5.28	0.35	C:\DATABASE\NBS75K.L			
			Butane, 2-methyl-	62518	000078-78-4	53
			Butane, 2-methyl-	62517	000078-78-4	53
			3-Buten-1-ol	62484	000627-27-0	25

12 5.44 0.12 C:\DATABASE\NBS75K.L
2-Butanamine 62534 013952-84-6 23
Diazene, dimethyl- 90 000503-28-6 9
2-Propanamine 62339 000075-31-0 9

13 5.52 0.04 C:\DATABASE\NBS75K.L
Acetone 62326 000067-64-1 9
Acetone 62322 000067-64-1 9
2-Pentanamine, 4-methyl- 1648 000108-09-8 9

14 5.85 0.16 C:\DATABASE\NBS75K.L
1-Pentene 230 000109-67-1 58
Cyclopropane, ethyl- 62460 001191-96-4 52
1-Pentene 62466 000109-67-1 52

15 6.38 0.17 C:\DATABASE\NBS75K.L
Pentane 62515 000109-66-0 53
Pentane 280 000109-66-0 50
Butane, 2-methyl- 62518 000078-78-4 37

16 6.64 0.17 C:\DATABASE\NBS75K.L
1,3-Butadiene, 2-methyl- 62407 000078-79-5 94
1,3-Butadiene, 2-methyl- 62408 000078-79-5 90
1,2-Pentadiene 181 000591-95-7 90

17 6.88 0.21 C:\DATABASE\NBS75K.L
1-Butene, 2-methyl- 62458 000563-46-2 60
2-Butene, 2-methyl- 62461 000513-35-9 58
2-Pentene 231 000109-68-2 58

18 7.37 0.18 C:\DATABASE\NBS75K.L
1-Butene, 2-methyl- 62457 000563-46-2 72
1-Butene, 2-methyl- 62458 000563-46-2 68
Cyclopropane, 1,2-dimethyl-, cis- 62467 000930-18-7 68

19 7.67 0.19 C:\DATABASE\NBS75K.L
2-Butene, 2-methyl- 62461 000513-35-9 70
Cyclopropane, 1,2-dimethyl-, cis- 62467 000930-18-7 68
Cyclopropane, 1,1-dimethyl- 62468 001630-94-0 59

20 8.55 0.29 C:\DATABASE\NBS75K.L
Butane, 2,2-dimethyl- 732 000075-83-2 72
Butane, 2,2-dimethyl- 62861 000075-83-2 72
Butane, 2,2-dimethyl- 62862 000075-83-2 53

21 9.46 0.23 C:\DATABASE\NBS75K.L
Cyclopentene 62412 000142-29-0 87
Cyclopentene 185 000142-29-0 87
Cyclopentene 62411 000142-29-0 86

22 9.77 0.27 C:\DATABASE\NBS75K.L
1-Pentene, 4-methyl- 599 000691-37-2 64
1-Propene, 2-methyl- 62304 000115-11-7 43
2-Butene, (E)- 62302 000624-64-6 43

23 10.04 0.21 C:\DATABASE\NBS75K.L
Cyclobutane, methyl- 229 000598-61-8 83
Cyclopentane 234 000287-92-3 80
1-Pentene 62464 000109-67-1 80

24 10.22 0.28 C:\DATABASE\NBS75K.L
Butane, 2,3-dimethyl- 62871 000079-29-8 78
Butane, 2,3-dimethyl- 62870 000079-29-8 78
Butane, 2,3-dimethyl- 62869 000079-29-8 72

25 10.50 0.32 C:\DATABASE\NBS75K.L
Pentane, 2-methyl- 733 000107-83-5 91
Pentane, 2-methyl- 62863 000107-83-5 91
Pentane, 2-methyl- 62865 000107-83-5 86

26 10.78 0.04 C:\DATABASE\NBS75K.L
Butanal 265 000123-72-8 90
Butanal 62487 000123-72-8 58
Butanal 62488 000123-72-8 53

27 11.21 0.31 C:\DATABASE\NBS75K.L
Pentane, 3-methyl- 62867 000096-14-0 87
Pentane, 3-methyl- 62868 000096-14-0 87
Hexane, 2,2,3-trimethyl- 5165 016747-25-4 56

28 11.47 0.24 C:\DATABASE\NBS75K.L
1-Pentene, 2-methyl- 598 000763-29-1 94
1-Pentene, 2-methyl- 62768 000763-29-1 94
Cyclohexane 62778 000110-82-7 83

29 12.05 0.30 C:\DATABASE\NBS75K.L
Hexane 62874 000110-54-3 86
Hexane 736 000110-54-3 64
Hexane 62872 000110-54-3 56

30 12.28 0.27 C:\DATABASE\NBS75K.L
2-Hexene 589 000592-43-8 90
2-Hexene, (E)- 62752 004050-45-7 90
2-Hexene, (E)- 62751 004050-45-7 90

31 12.68 0.28 C:\DATABASE\NBS75K.L
2-Hexene 589 000592-43-8 90
2-Hexene, (E)- 62751 004050-45-7 90
2-Hexene, (Z)- 583 007688-21-3 90

32 13.16 0.30 C:\DATABASE\NBS75K.L
Cyclopentane, methyl- 594 000096-37-7 90
Cyclohexane 62778 000110-82-7 72
Cyclobutane, ethyl- 604 004806-61-5 72

33 13.37 0.39 C:\DATABASE\NBS75K.L
Pentane, 2,4-dimethyl- 63424 000108-08-7 91
Pentane, 2,4-dimethyl- 1594 000108-08-7 90
Pentane, 2,4-dimethyl- 63425 000108-08-7 86

34 14.13 0.36 C:\DATABASE\NBS75K.L
Benzene 62628 000071-43-2 94
1,3-Hexadien-5-yne 404 010420-90-3 94
Benzene 62627 000071-43-2 91

35 14.48 0.42 C:\DATABASE\NBS75K.L
Cyclohexane 62777 000110-82-7 91
Cyclohexane 62779 000110-82-7 90
Cyclohexane 62776 000110-82-7 90

36 14.85 0.54 C:\DATABASE\NBS75K.L
Hexane, 2-methyl- 63435 000591-76-4 90
Hexane, 2-methyl- 63434 000591-76-4 86
Hexane, 2-methyl- 63433 000591-76-4 86

37 14.91 0.54 C:\DATABASE\NBS75K.L
Pentane, 2,3-dimethyl- 63430 000565-59-3 91
Pentane, 2,3-dimethyl- 63432 000565-59-3 78
Pentane, 2,3-dimethyl- 1597 000565-59-3 72

38 15.17 0.55 C:\DATABASE\NBS75K.L
Hexane, 3-methyl- 63422 000589-34-4 83
Heptane, 3,4-dimethyl- 65136 000922-28-1 72
Hexane, 3-methyl- 1593 000589-34-4 72

39 15.64 0.75 C:\DATABASE\NBS75K.L
Heptane, 2,2,4,6,6-pentamethyl- 68260 013475-82-6 78
Pentane, 2,2,4-trimethyl- 64220 000540-84-1 78
Hexane, 2,2-dimethyl- 64216 000590-73-8 72

40 15.92 1.30 C:\DATABASE\NBS75K.L

Benzene, methyl-, trifluoro deriv. 8769 027359-10-0 96
Benzene, (trifluoromethyl)- 66428 000098-08-8 94
Benzene, (trifluoromethyl)- 8768 000098-08-8 93

41 16.01 0.52 C:\DATABASE\NBS75K.L
Heptane 63438 000142-82-5 94
Heptane 63440 000142-82-5 93
Heptane 1600 000142-82-5 91

42 16.70 0.56 C:\DATABASE\NBS75K.L
Cyclohexane, methyl- 63236 000108-87-2 96
Cyclohexane, methyl- 1326 000108-87-2 94
Cyclohexane, methyl- 63235 000108-87-2 93

43 17.63 0.69 C:\DATABASE\NBS75K.L
Pentane, 2,3,4-trimethyl- 3100 000565-75-3 91
Pentane, 2,3,4-trimethyl- 64228 000565-75-3 90
Pentane, 2,3,4-trimethyl- 64229 000565-75-3 83

44 17.77 0.51 C:\DATABASE\NBS75K.L
Toluene 63028 000108-88-3 97
Toluene 63029 000108-88-3 94
Toluene 63030 000108-88-3 94

45 18.07 0.74 C:\DATABASE\NBS75K.L
Heptane, 2-methyl- 3092 000592-27-8 91
Heptane, 2-methyl- 64218 000592-27-8 90
1-Propanol, 2,2-dimethyl-, propano 8370 003581-69-9 59

46 18.29 0.71 C:\DATABASE\NBS75K.L
Heptane, 3-methyl- 3099 000589-81-1 90
Pentane, 2,4-dimethyl- 1594 000108-08-7 64
Pentane, 2,4-dimethyl- 63425 000108-08-7 64

47 18.99 0.70 C:\DATABASE\NBS75K.L
Octane 64209 000111-65-9 94
Octane 3084 000111-65-9 90
Octane 64207 000111-65-9 87

48 20.41 0.60 C:\DATABASE\NBS75K.L
Ethylbenzene 63690 000100-41-4 94
Ethylbenzene 2026 000100-41-4 94
Ethylbenzene 63691 000100-41-4 91

49 20.64 1.14 C:\DATABASE\NBS75K.L
p-Xylene 63699 000106-42-3 97
Benzene, 1,2-dimethyl- 63707 000095-47-6 97
p-Xylene 63700 000106-42-3 95

50 21.13 0.39 C:\DATABASE\NBS75K.L
Styrene 63645 000100-42-5 97
Styrene 63646 000100-42-5 95
1,3,5,7-Cyclooctatetraene 1949 000629-20-9 95

51 21.28 0.58 C:\DATABASE\NBS75K.L
Benzene, 1,3-dimethyl- 63695 000108-38-3 97
p-Xylene 63702 000106-42-3 95
Benzene, 1,2-dimethyl- 63706 000095-47-6 95

52 21.64 0.85 C:\DATABASE\NBS75K.L
Nonane 65144 000111-84-2 91
Nonane 65142 000111-84-2 90
Nonane 65145 000111-84-2 64

53 21.93 0.24 C:\DATABASE\NBS75K.L
Benzene, 1-bromo-3-fluoro- 16034 001073-06-9 94
Benzene, 1-bromo-2-fluoro- 16035 001072-85-1 94
Benzene, 1-bromo-2-fluoro- 68408 001072-85-1 94

54 22.15 0.70 C:\DATABASE\NBS75K.L
Benzene, (1-methylethyl)- 3763 000098-82-8 95

Benzene, (1-methylethyl)- 64554 000098-82-8 94
Benzene, (1-methylethyl)- 64556 000098-82-8 91

55 22.50 0.03 C:\DATABASE\NBS75K.L
Phenol, 2-[(dimethylamino)methyl]- 17483 055955-99-2 28
Pyridinium, 1-(carboxymethyl)-, hy 6736 024608-93-3 25
Phenol, 4-(2-aminopropyl)-, (.+/-. 10013 001518-86-1 9

56 22.71 0.04 C:\DATABASE\NBS75K.L
Benzaldehyde 63685 000100-52-7 96
Benzaldehyde 63688 000100-52-7 96
Benzaldehyde 63689 000100-52-7 96

57 22.76 0.22 C:\DATABASE\NBS75K.L
.alpha.-Pinene 65808 000080-56-8 93
Bicyclo[3.1.1]hept-2-ene, 3,6,6-tr 6692 004889-83-2 87
.alpha.-Pinene 65809 000080-56-8 87

58 22.97 0.68 C:\DATABASE\NBS75K.L
Benzene, propyl- 64582 000103-65-1 91
Benzene, propyl- 64583 000103-65-1 91
Benzene, propyl- 3781 000103-65-1 91

59 23.13 0.04 C:\DATABASE\NBS75K.L
Bicyclo[2.2.1]heptane, 7,7-dimethy 6625 000471-84-1 98
Bicyclo[2.2.1]heptane, 7,7-dimethy 65761 000471-84-1 92
Bicyclo[2.2.1]heptane, 2,2-dimethy 6695 005794-03-6 58

60 23.20 0.26 C:\DATABASE\NBS75K.L
Camphene 65764 000079-92-5 98
Camphene 65765 000079-92-5 98
Camphene 65767 000079-92-5 97

61 23.37 0.61 C:\DATABASE\NBS75K.L
Benzene, 1,2,3-trimethyl- 64572 000526-73-8 95
Benzene, 1,3,5-trimethyl- 64568 000108-67-8 95
Benzene, 1,2,3-trimethyl- 64573 000526-73-8 95

62 24.13 0.65 C:\DATABASE\NBS75K.L
Benzene, 1,3,5-trimethyl- 64571 000108-67-8 97
Benzene, 1,2,3-trimethyl- 64572 000526-73-8 95
Benzene, 1,2,4-trimethyl- 64578 000095-63-6 95

63 25.01 0.15 C:\DATABASE\NBS75K.L
Benzene, 1-methyl-4-(1-methylethyl 6201 000099-87-6 97
Benzene, 1-methyl-2-(1-methylethyl 6228 000527-84-4 97
Benzene, 1-methyl-3-(1-methylethyl 65579 000535-77-3 95

64 25.32 0.18 C:\DATABASE\NBS75K.L
D-Limonene 65790 005989-27-5 95
D-Limonene 6664 005989-27-5 94
Limonene 6647 000138-86-3 90

65 25.76 0.05 C:\DATABASE\NBS75K.L
Acetophenone 64533 000098-86-2 94
Acetophenone 3752 000098-86-2 81
Acetophenone 64537 000098-86-2 81

66 25.95 0.05 C:\DATABASE\NBS75K.L
Ethane, 1,1,2-trichloro-1,2,2-trif 69052 000076-13-1 40
Ethane, 1,1,2,2-tetrachloro-1-fluo 18640 000354-14-3 40
Ethane, 1,1,2-trichloro-1,2,2-trif 69051 000076-13-1 38

67 26.87 0.07 C:\DATABASE\NBS75K.L
o-Isopropenyltoluene 5877 007399-49-7 98
Benzene, 1-methyl-4-(1-methylethen 5874 001195-32-0 98
Benzene, 1-methyl-4-(1-methylethen 65410 001195-32-0 93

68 27.36 0.07 C:\DATABASE\NBS75K.L
Butane, 1,1,3,4-tetrachloro-1,2,2, 42990 000423-38-1 50
Butane, trichloroheptafluoro- 40359 028984-80-7 43

Hexane, heptachlorohexafluoro- 56031 072101-28-1 38

69 27.39 0.08 C:\DATABASE\NBS75K.L
Butane, 1,1,3,4-tetrachloro-1,2,2, 42990 000423-38-1 53
Butane, 1,2,3,4-tetrachloro-1,1,2, 42989 000375-45-1 43
Ethane, 1,1,2-trichloro-1,2,2-trif 69052 000076-13-1 38

70 27.61 0.03 C:\DATABASE\NBS75K.L
Ethane, 1,1,2-trichloro-1,2,2-trif 69052 000076-13-1 59
Ethane, 1,1,2,2-tetrachloro-1-fluo 18640 000354-14-3 47
Ethane, 1,1,2-trichloro-1,2,2-trif 69051 000076-13-1 40

Information from Data File:
File: C:\SARAH\SC2-2.D
Operator:
Date Acquired: 2 Nov 1998 2:51 pm
Method File: TO15D
Sample Name: smog chamber 548 10-24-98
Misc Info:
Vial Number: 1

Search Libraries: C:\DATABASE\NBS75K.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - VOCS.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	0.24	0.08	C:\DATABASE\NBS75K.L			
			Acetic acid, oxo-	305	000298-12-4	3
			Ethane	62248	000074-84-0	2
			Ethane	62247	000074-84-0	2
2	0.47	0.03	C:\DATABASE\NBS75K.L			
			Piperidine, 1-nitro-	5328	007119-94-0	4
			Ethane	62246	000074-84-0	2
			Ethane	11	000074-84-0	2
3	0.66	0.05	C:\DATABASE\NBS75K.L			
			Piperidine, 1-nitro-	5328	007119-94-0	4
			Ethane	62248	000074-84-0	2
			Ethane	62247	000074-84-0	2
4	2.70	23.17	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	4
			Ethylene oxide	62266	000075-21-8	4
			Acetaldehyde	62265	000075-07-0	3
5	2.81	0.57	C:\DATABASE\NBS75K.L			
			Carbon dioxide	34	000124-38-9	3
			Ethylene oxide	62267	000075-21-8	3
			Carbon dioxide	62263	000124-38-9	3
6	2.93	61.45	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	4
			Ethylene oxide	62266	000075-21-8	4
			Acetaldehyde	62265	000075-07-0	3
7	3.37	1.88	C:\DATABASE\NBS75K.L			
			Dichlorotetrafluoroethane	68163	000076-14-2	68
			Dichlorotetrafluoroethane	14961	000076-14-2	53
			Dichlorodifluoromethane	64510	000075-71-8	22
8	3.60	0.05	C:\DATABASE\NBS75K.L			
			Carbon dioxide	34	000124-38-9	4
			Carbon dioxide	62263	000124-38-9	4
			1,3-Cyclohexanediol	3291	000504-01-8	4
9	3.67	0.05	C:\DATABASE\NBS75K.L			
			Ethyne, fluoro-	35	002713-09-9	5
			Acetaldehyde	36	000075-07-0	4

Carbon dioxide 62263 000124-38-9 4

10 3.72 0.19 C:\DATABASE\NBS75K.L
1-Methyl-2-phenoxyethylamine 10031 035205-54-0 9
Acetaldehyde 62264 000075-07-0 7
Carbon dioxide 62263 000124-38-9 4

11 5.27 0.26 C:\DATABASE\NBS75K.L
Butane, 2-methyl- 62518 000078-78-4 47
Butane, 2-methyl- 62517 000078-78-4 46
Oxirane, 2,2-dimethyl- 62511 000558-30-5 35

12 5.44 0.15 C:\DATABASE\NBS75K.L
Acetone 62325 000067-64-1 17
Propylene oxide 62320 000075-56-9 9
Trimethylene oxide 62318 000503-30-0 9

13 5.54 0.89 C:\DATABASE\NBS75K.L
Acetone 62326 000067-64-1 72
Acetone 62325 000067-64-1 64
Acetone 62324 000067-64-1 64

14 6.36 0.12 C:\DATABASE\NBS75K.L
Pentane 280 000109-66-0 43
Butane, 2-methyl- 62518 000078-78-4 12
3-Buten-1-ol 62483 000627-27-0 9

15 8.52 0.22 C:\DATABASE\NBS75K.L
Butane, 2,2-dimethyl- 62861 000075-83-2 72
Butane, 2,2-dimethyl- 732 000075-83-2 72
Butane, 2,2-dimethyl- 62862 000075-83-2 56

16 9.75 0.04 C:\DATABASE\NBS75K.L
2-Butenal 62440 004170-30-3 38
2-Propenal, 2-methyl- 62429 000078-85-3 35
Cyclopropyl carbinol 268 002516-33-8 23

17 10.02 0.12 C:\DATABASE\NBS75K.L
Cyclopropane, ethyl- 227 001191-96-4 76
1-Pentene 62466 000109-67-1 64
Cyclobutane, methyl- 229 000598-61-8 64

18 10.19 0.18 C:\DATABASE\NBS75K.L
Butane, 2,3-dimethyl- 62870 000079-29-8 80
Butane, 2,3-dimethyl- 735 000079-29-8 64
Butane, 2,3-dimethyl- 62869 000079-29-8 64

19 10.46 0.17 C:\DATABASE\NBS75K.L
Pentane, 2-methyl- 733 000107-83-5 87
Pentane, 2-methyl- 62863 000107-83-5 83
Pentane, 2-methyl- 62865 000107-83-5 80

20 10.57 0.05 C:\DATABASE\NBS75K.L
2-Butene, 2-methyl- 62462 000513-35-9 43
3-Buten-2-one 62447 000078-94-4 38
1-Butene, 2-methyl- 62458 000563-46-2 35

21 10.65 0.04 C:\DATABASE\NBS75K.L
2-Pentanone 706 000107-87-9 9
2-Pentanone 62837 000107-87-9 9
2-Butanone, 3-methyl- 703 000563-80-4 9

22 10.78 0.12 C:\DATABASE\NBS75K.L
Butanal 62486 000123-72-8 91
Butanal 265 000123-72-8 90
Butanal 62489 000123-72-8 90

23 11.10 0.38 C:\DATABASE\NBS75K.L
2-Butanone 62493 000078-93-3 59
2-Butanone 62491 000078-93-3 59
2-Butanone 62492 000078-93-3 59

24 12.01 0.15 C:\DATABASE\NBS75K.L
Hexane 62874 000110-54-3 58
Hexane 62872 000110-54-3 58
Hexane 62873 000110-54-3 58

25 13.13 0.13 C:\DATABASE\NBS75K.L
Cyclopentane, methyl- 594 000096-37-7 62
Cyclopentane, methyl- 62763 000096-37-7 53
Cyclobutane, ethyl- 604 004806-61-5 47

26 13.37 0.20 C:\DATABASE\NBS75K.L
Pentane, 2,4-dimethyl- 63424 000108-08-7 64
Pentane, 2,4-dimethyl- 1594 000108-08-7 64
Heptane, 3-methyl- 3099 000589-81-1 53

27 13.94 0.07 C:\DATABASE\NBS75K.L
2-Butanone, 3-methyl- 703 000563-80-4 38
2-Pentanone 62835 000107-87-9 35
2-Pentanone 62837 000107-87-9 35

28 14.14 0.47 C:\DATABASE\NBS75K.L
Benzene 62627 000071-43-2 94
1,3-Hexadien-5-yne 404 010420-90-3 91
Benzene 62628 000071-43-2 91

29 14.26 0.04 C:\DATABASE\NBS75K.L
Acetamide, N-[(8.alpha.,9R)-9-hydr 52279 056847-12-2 38
2-Pentanamine 768 000625-30-9 33
1-Methyl-2-phenoxyethylamine 10031 035205-54-0 33

30 14.47 0.19 C:\DATABASE\NBS75K.L
Cyclohexane 62778 000110-82-7 81
Cyclohexane 62777 000110-82-7 81
Cyclohexane 606 000110-82-7 76

31 14.86 0.26 C:\DATABASE\NBS75K.L
Hexane, 2-methyl- 63434 000591-76-4 64
Hexane, 2-methyl- 63433 000591-76-4 64
Hexane, 2-methyl- 63435 000591-76-4 58

32 14.92 0.42 C:\DATABASE\NBS75K.L
Pentane, 2,3-dimethyl- 63429 000565-59-3 47
Propane, 1-isocyanato-2-methyl- 1400 001873-29-6 45
Pentane, 2,3-dimethyl- 63431 000565-59-3 43

33 15.17 0.29 C:\DATABASE\NBS75K.L
Hexane, 3-methyl- 63421 000589-34-4 81
Hexane, 3-methyl- 63423 000589-34-4 81
Hexane, 3-methyl- 1593 000589-34-4 72

34 15.29 0.03 C:\DATABASE\NBS75K.L
3-Pentanone 723 000096-22-0 10
Butanal, 2-methyl- 62844 000096-17-3 9
1-Pentene, 4,4-dimethyl- 63226 000762-62-9 9

35 15.65 0.50 C:\DATABASE\NBS75K.L
Hexane, 2,2-dimethyl- 64216 000590-73-8 78
Pentane, 2,2,4-trimethyl- 64220 000540-84-1 78
Hexane, 2,2,4-trimethyl- 65103 016747-26-5 64

36 15.93 1.77 C:\DATABASE\NBS75K.L
Benzene, methyl-, trifluoro deriv. 8769 027359-10-0 96
Benzene, (trifluoromethyl)- 8768 000098-08-8 95
Benzene, (trifluoromethyl)- 66428 000098-08-8 94

37 16.01 0.19 C:\DATABASE\NBS75K.L
Heptane 63438 000142-82-5 64
Heptane 63440 000142-82-5 62
Heptane 63439 000142-82-5 58

38 16.36 0.04 C:\DATABASE\NBS75K.L
2-Hexanamine, 5-methyl- 3163 028292-43-5 4
L-Alanine, 1,1-dimethylethyl ester 17987 013404-22-3 4
Acetamide, 2-cyano- 532 000107-91-5 4

39 16.71 0.19 C:\DATABASE\NBS75K.L
Cyclohexane, methyl- 63236 000108-87-2 95
Cyclohexane, methyl- 1326 000108-87-2 94
Cyclohexane, methyl- 63235 000108-87-2 93

40 17.15 0.04 C:\DATABASE\NBS75K.L
1-Octadecanamine, N-methyl- 40007 002439-55-6 39
Propanamide 62531 000079-05-0 9
Ethyne, fluoro- 35 002713-09-9 4

41 17.63 0.33 C:\DATABASE\NBS75K.L
Pentane, 2,3,4-trimethyl- 3100 000565-75-3 72
Pentane, 3-ethyl- 1595 000617-78-7 59
Pentane, 2,3,4-trimethyl- 64229 000565-75-3 56

42 17.77 0.46 C:\DATABASE\NBS75K.L
Toluene 63028 000108-88-3 95
Toluene 965 000108-88-3 93
Toluene 63029 000108-88-3 93

43 18.07 0.32 C:\DATABASE\NBS75K.L
Heptane, 2-methyl- 3092 000592-27-8 87
Heptane, 2-methyl- 64218 000592-27-8 76
Hexane, 2,5-dimethyl- 64206 000592-13-2 64

44 18.28 0.25 C:\DATABASE\NBS75K.L
Heptane, 3-methyl- 64227 000589-81-1 76
Heptane, 3-methyl- 3099 000589-81-1 59
Hexane, 2,4-dimethyl- 64213 000589-43-5 52

45 18.42 0.04 C:\DATABASE\NBS75K.L
Hexanal 63408 000066-25-1 38
Hexanal 1573 000066-25-1 23
Hexanal 63410 000066-25-1 17

46 18.99 0.22 C:\DATABASE\NBS75K.L
Octane 64207 000111-65-9 74
Octane 3084 000111-65-9 74
Decane, 5,6-dimethyl- 15355 001636-43-7 53

47 20.41 0.43 C:\DATABASE\NBS75K.L
Ethylbenzene 63690 000100-41-4 93
Ethylbenzene 2026 000100-41-4 93
Ethylbenzene 63691 000100-41-4 90

48 20.65 0.38 C:\DATABASE\NBS75K.L
p-Xylene 63702 000106-42-3 95
Benzene, 1,2-dimethyl- 63707 000095-47-6 94
Benzene, 1,3-dimethyl- 63695 000108-38-3 94

49 21.28 0.25 C:\DATABASE\NBS75K.L
Benzene, 1,2-dimethyl- 63705 000095-47-6 94
Benzene, 1,2-dimethyl- 63706 000095-47-6 94
Benzene, 1,2-dimethyl- 63707 000095-47-6 94

50 21.64 0.21 C:\DATABASE\NBS75K.L
Nonane 65144 000111-84-2 87
Nonane 65142 000111-84-2 87
Undecane 67317 001120-21-4 59

51 21.93 0.29 C:\DATABASE\NBS75K.L
Benzene, 1-bromo-3-fluoro- 16034 001073-06-9 95
Benzene, 1-bromo-3-fluoro- 68407 001073-06-9 93
Benzene, 1-bromo-2-fluoro- 68408 001072-85-1 91

52 22.15 0.47 C:\DATABASE\NBS75K.L

Benzene, (1-methylethyl)- 3763 000098-82-8 94
Benzene, (1-methylethyl)- 64554 000098-82-8 93
Benzene, (1-methylethyl)- 64555 000098-82-8 90

53 22.70 0.25 C:\DATABASE\NBS75K.L
Benzaldehyde 63688 000100-52-7 97
Benzaldehyde 63689 000100-52-7 96
Benzaldehyde 2020 000100-52-7 93

54 22.98 0.37 C:\DATABASE\NBS75K.L
Benzene, propyl- 64583 000103-65-1 91
Benzene, propyl- 64584 000103-65-1 91
Benzene, propyl- 64582 000103-65-1 90

55 24.14 0.09 C:\DATABASE\NBS75K.L
Benzene, 1,2,4-trimethyl- 3775 000095-63-6 86
Benzene, 1-ethyl-3-methyl- 64565 000620-14-4 83
1,2,4-Trimethylbenzene 3771 000095-36-3 64

56 25.76 0.10 C:\DATABASE\NBS75K.L
Acetophenone 64537 000098-86-2 93
Acetophenone 3752 000098-86-2 90
Acetophenone 64534 000098-86-2 90

57 25.94 0.07 C:\DATABASE\NBS75K.L
Ethane, 1,1,2-trichloro-1,2,2-trif 69052 000076-13-1 56
Ethane, 1,1,2-trichloro-1,2,2-trif 69051 000076-13-1 40
Ethane, 1,1,2-trichloro-1,2,2-trif 69050 000076-13-1 38

58 27.39 0.18 C:\DATABASE\NBS75K.L
Butane, trichloroheptafluoro- 40359 028984-80-7 38
Ethane, 1,1,2-trichloro-1,2,2-trif 69052 000076-13-1 38
Butane, 1,2,3,4-tetrachloro-1,1,2, 42989 000375-45-1 38

59 27.62 0.03 C:\DATABASE\NBS75K.L
Ethane, 1,1,2-trichloro-1,2,2-trif 69050 000076-13-1 38
Ethane, 1,1,2-trichloro-1,2,2-trif 69051 000076-13-1 37
Ethane, 1,1,2-trichloro-1,2,2-trif 19234 000076-13-1 25

Sun Jun 27 16:58:22 1999

Information from Data File:
File: C:\SARAH\SC3-1.D
Operator:
Date Acquired: 3 Nov 1998 1:43 pm
Method File: TO15D
Sample Name: SC3-1.D
Misc Info:
Vial Number: 1

Search Libraries: C:\DATABASE\NBS75K.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - VOCS.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	0.56	0.03	C:\DATABASE\NBS75K.L			
			Piperidine, 1-nitro-	5328	007119-94-0	4
			Ethane	11	000074-84-0	2
			Formaldehyde	10	000050-00-0	2
2	2.71	16.98	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	4
			Ethylene oxide	62266	000075-21-8	4
			Acetaldehyde	62265	000075-07-0	3
3	2.82	9.02	C:\DATABASE\NBS75K.L			
			Carbon dioxide	34	000124-38-9	3
			Ethylene oxide	62267	000075-21-8	3
			Carbon dioxide	62263	000124-38-9	3
4	2.93	51.88	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	4
			Ethylene oxide	62266	000075-21-8	4
			Acetaldehyde	62265	000075-07-0	3
5	3.37	3.54	C:\DATABASE\NBS75K.L			
			Dichlorotetrafluoroethane	68163	000076-14-2	62
			Dichlorotetrafluoroethane	14961	000076-14-2	50
			Dichlorodifluoromethane	64510	000075-71-8	27
6	3.61	0.36	C:\DATABASE\NBS75K.L			
			1,3-Cyclohexanediol	3291	000504-01-8	9
			Carbon dioxide	34	000124-38-9	4
			Carbon dioxide	62263	000124-38-9	4
7	3.72	0.23	C:\DATABASE\NBS75K.L			
			Butane	62336	000106-97-8	10
			Butane	99	000106-97-8	10
			1-Methyl-2-phenoxyethylamine	10031	035205-54-0	9
8	3.86	0.14	C:\DATABASE\NBS75K.L			
			Carbon dioxide	62263	000124-38-9	4
			Carbon dioxide	34	000124-38-9	4
			Ethylene oxide	62267	000075-21-8	3
9	4.09	0.12	C:\DATABASE\NBS75K.L			
			2-Oxetanone, 4,4-dimethyl-	1450	001823-52-5	50
			1-Propene, 2-methyl-	62305	000115-11-7	35
			1-Butene	62307	000106-98-9	20
10	4.76	0.16	C:\DATABASE\NBS75K.L			
			1-Butene, 3-methyl-	236	000563-45-1	58
			1-Butene, 2-methyl-	62457	000563-46-2	58
			1-Butene, 2-methyl-	225	000563-46-2	49
11	5.28	0.25	C:\DATABASE\NBS75K.L			
			Butane, 2-methyl-	62518	000078-78-4	64
			Butane, 2-methyl-	62517	000078-78-4	64
			Butane, 2-methyl-	281	000078-78-4	42

12 5.51 0.46 C:\DATABASE\NBS75K.L
Acetone 62325 000067-64-1 64
Acetone 62323 000067-64-1 42
Acetone 62324 000067-64-1 42

13 5.84 0.13 C:\DATABASE\NBS75K.L
1-Pentene 230 000109-67-1 58
1-Pentene 62466 000109-67-1 52
Cyclopropane, ethyl- 227 001191-96-4 52

14 6.38 0.12 C:\DATABASE\NBS75K.L
Pentane 280 000109-66-0 58
Pentane 62515 000109-66-0 50
Pentane 62516 000109-66-0 50

15 6.64 0.11 C:\DATABASE\NBS75K.L
1,3-Butadiene, 2-methyl- 184 000078-79-5 91
1,3-Butadiene, 2-methyl- 62410 000078-79-5 91
1,3-Butadiene, 2-methyl- 62409 000078-79-5 87

16 6.88 0.13 C:\DATABASE\NBS75K.L
2-Pentene, (Z)- 62456 000627-20-3 64
Cyclopropane, 1,2-dimethyl-, cis- 62467 000930-18-7 53
1-Butene, 2-methyl- 62457 000563-46-2 52

17 7.36 0.12 C:\DATABASE\NBS75K.L
2-Pentene, (Z)- 62456 000627-20-3 64
2-Pentene, (E)- 233 000646-04-8 53
Cyclopropane, 1,2-dimethyl-, cis- 62467 000930-18-7 52

18 7.67 0.13 C:\DATABASE\NBS75K.L
Cyclopropane, 1,2-dimethyl-, cis- 62467 000930-18-7 53
2-Butene, 2-methyl- 62461 000513-35-9 53
Cyclopropane, 1,1-dimethyl- 235 001630-94-0 53

19 7.99 0.03 C:\DATABASE\NBS75K.L
Acetamide 62338 000060-35-5 9
3-Pentanol 62943 000584-02-1 9
2-Propanol, 2-methyl- 62574 000075-65-0 9

20 8.53 0.20 C:\DATABASE\NBS75K.L
Butane, 2,2-dimethyl- 732 000075-83-2 72
Butane, 2,2-dimethyl- 62862 000075-83-2 64
Butane, 2,2-dimethyl- 62861 000075-83-2 64

21 9.46 0.15 C:\DATABASE\NBS75K.L
Cyclopentene 185 000142-29-0 93
Cyclopentene 62411 000142-29-0 87
Cyclopentene 62412 000142-29-0 83

22 9.77 0.19 C:\DATABASE\NBS75K.L
1-Pentene, 4-methyl- 599 000691-37-2 58
1-Propene, 2-methyl- 62304 000115-11-7 43
1-Pentene, 2-methyl- 62768 000763-29-1 42

23 10.03 0.15 C:\DATABASE\NBS75K.L
1-Pentene 62464 000109-67-1 83
Cyclobutane, methyl- 229 000598-61-8 80
1-Pentene 62466 000109-67-1 72

24 10.21 0.19 C:\DATABASE\NBS75K.L
Butane, 2,3-dimethyl- 62871 000079-29-8 80
Butane, 2,3-dimethyl- 62870 000079-29-8 72
Butane, 2,3-dimethyl- 62869 000079-29-8 50

25 10.48 0.22 C:\DATABASE\NBS75K.L
Pentane, 2-methyl- 62863 000107-83-5 91
Pentane, 2-methyl- 733 000107-83-5 90
Pentane, 2-methyl- 62865 000107-83-5 87

26 10.76 0.76 C:\DATABASE\NBS75K.L
Butanal 62486 000123-72-8 91
Butanal 62490 000123-72-8 91
Butanal 62487 000123-72-8 90

27 11.21 0.36 C:\DATABASE\NBS75K.L
Hexane 736 000110-54-3 64
Pentane, 2,2,4,4-tetramethyl- 5133 001070-87-7 64
Propanal, 2,2-dimethyl- 715 000630-19-3 43

28 11.46 0.17 C:\DATABASE\NBS75K.L
1-Pentene, 2-methyl- 62768 000763-29-1 93
1-Pentene, 2-methyl- 62769 000763-29-1 80
1-Pentene, 2-methyl- 598 000763-29-1 80

29 12.04 0.21 C:\DATABASE\NBS75K.L
Hexane 736 000110-54-3 58
Hexane 62874 000110-54-3 58
Hexane 62872 000110-54-3 58

30 12.27 0.19 C:\DATABASE\NBS75K.L
2-Hexene, (E)- 585 004050-45-7 86
2-Hexene, (E)- 62752 004050-45-7 81
2-Hexene 589 000592-43-8 76

31 12.68 0.19 C:\DATABASE\NBS75K.L
2-Hexene 589 000592-43-8 93
2-Hexene, (E)- 62752 004050-45-7 87
2-Hexene, (E)- 62751 004050-45-7 87

32 13.15 0.21 C:\DATABASE\NBS75K.L
Cyclopentane, methyl- 594 000096-37-7 90
Cyclopentane, methyl- 62763 000096-37-7 80
Cyclohexane 62777 000110-82-7 72

33 13.23 0.06 C:\DATABASE\NBS75K.L
2-Butenal 62440 004170-30-3 90
Furan, 2,3-dihydro- 62438 001191-99-7 90
2-Butenal 62442 004170-30-3 90

34 13.37 0.25 C:\DATABASE\NBS75K.L
Pentane, 2,4-dimethyl- 63425 000108-08-7 80
Pentane, 2,4-dimethyl- 1594 000108-08-7 80
Pentane, 2,4-dimethyl- 63424 000108-08-7 58

35 13.95 0.03 C:\DATABASE\NBS75K.L
Piperazine 62810 000110-85-0 50
2-Butanone, 3-methyl- 703 000563-80-4 14
2-Pentanone 62837 000107-87-9 10

36 14.13 0.24 C:\DATABASE\NBS75K.L
Benzene 62628 000071-43-2 94
1,3-Hexadien-5-yne 404 010420-90-3 91
Benzene 62626 000071-43-2 91

37 14.48 0.31 C:\DATABASE\NBS75K.L
Cyclohexane 62776 000110-82-7 90
Cyclohexane 62777 000110-82-7 90
Cyclohexane 606 000110-82-7 90

38 14.86 0.38 C:\DATABASE\NBS75K.L
Hexane, 2-methyl- 63435 000591-76-4 90
Hexane, 2-methyl- 1598 000591-76-4 87
Oxirane, 2-methyl-3-propyl-, cis- 1531 006124-90-9 59

39 14.91 0.37 C:\DATABASE\NBS75K.L
Pentane, 2,3-dimethyl- 63429 000565-59-3 91
Pentane, 2,3-dimethyl- 63430 000565-59-3 91
Pentane, 2,3-dimethyl- 63432 000565-59-3 78

40 15.17 0.42 C:\DATABASE\NBS75K.L

Hexane, 3-methyl- 1593 000589-34-4 86
Hexane, 3-methyl- 63422 000589-34-4 80
Hexane, 3-methyl- 63421 000589-34-4 64

41 15.64 0.53 C:\DATABASE\NBS75K.L
Pentane, 2,2,4-trimethyl- 64221 000540-84-1 78
Hexane, 2,2-dimethyl- 64216 000590-73-8 78
Heptane, 2,2,4,6,6-pentamethyl- 68260 013475-82-6 78

42 15.92 1.32 C:\DATABASE\NBS75K.L
Benzene, methyl-, trifluoro deriv. 8769 027359-10-0 96
Benzene, (trifluoromethyl)- 8768 000098-08-8 95
Benzene, (trifluoromethyl)- 66428 000098-08-8 94

43 16.01 0.39 C:\DATABASE\NBS75K.L
Heptane 63438 000142-82-5 93
Heptane 63440 000142-82-5 90
Heptane 1600 000142-82-5 87

44 16.36 0.14 C:\DATABASE\NBS75K.L
1-Pentene, 2,4,4-trimethyl- 2693 000107-39-1 62
1-Pentene, 2,4,4-trimethyl- 64024 000107-39-1 58
2-Hexene, 5,5-dimethyl-, (Z)- 64046 039761-61-0 53

45 16.70 0.37 C:\DATABASE\NBS75K.L
Cyclohexane, methyl- 63236 000108-87-2 96
Cyclohexane, methyl- 1326 000108-87-2 94
Cyclohexane, methyl- 63235 000108-87-2 93

46 17.63 0.47 C:\DATABASE\NBS75K.L
Pentane, 2,3,4-trimethyl- 3100 000565-75-3 91
Pentane, 2,3,4-trimethyl- 64228 000565-75-3 86
Hexane, 3,3,4-trimethyl- 5135 016747-31-2 72

47 17.77 0.33 C:\DATABASE\NBS75K.L
Toluene 63028 000108-88-3 94
Toluene 965 000108-88-3 93
Toluene 63029 000108-88-3 93

48 18.06 0.75 C:\DATABASE\NBS75K.L
Heptane, 2-methyl- 3092 000592-27-8 59
Heptane, 2-methyl- 64218 000592-27-8 58
Hexane, 2,5-dimethyl- 64205 000592-13-2 53

49 18.28 0.48 C:\DATABASE\NBS75K.L
Heptane, 3-methyl- 3099 000589-81-1 81
Pentane, 2,4-dimethyl- 1594 000108-08-7 64
Pentane, 2,4-dimethyl- 63425 000108-08-7 64

50 18.42 0.07 C:\DATABASE\NBS75K.L
Hexanal 63408 000066-25-1 59
Hexanal 63410 000066-25-1 53
Hexanal 1573 000066-25-1 53

51 18.99 0.47 C:\DATABASE\NBS75K.L
Octane 64207 000111-65-9 87
Octane 3084 000111-65-9 87
Octane 64209 000111-65-9 81

52 20.41 0.39 C:\DATABASE\NBS75K.L
Ethylbenzene 2026 000100-41-4 94
Ethylbenzene 63690 000100-41-4 94
Ethylbenzene 63693 000100-41-4 91

53 20.65 0.73 C:\DATABASE\NBS75K.L
p-Xylene 63702 000106-42-3 95
Benzene, 1,2-dimethyl- 63705 000095-47-6 94
Benzene, 1,3-dimethyl- 2027 000108-38-3 94

54 21.13 0.34 C:\DATABASE\NBS75K.L
Styrene 63646 000100-42-5 94

Styrene 63645 000100-42-5 94
1,3,5,7-Cyclooctatetraene 1949 000629-20-9 93

55 21.27 0.38 C:\DATABASE\NBS75K.L
Benzene, 1,2-dimethyl- 63706 000095-47-6 94
Benzene, 1,2-dimethyl- 63705 000095-47-6 94
Benzene, 1,3-dimethyl- 63695 000108-38-3 94

56 21.64 0.56 C:\DATABASE\NBS75K.L
Nonane 65142 000111-84-2 90
Nonane 65145 000111-84-2 90
Nonane 65144 000111-84-2 87

57 21.93 0.24 C:\DATABASE\NBS75K.L
Benzene, 1-bromo-3-fluoro- 16034 001073-06-9 97
Benzene, 1-bromo-3-fluoro- 68407 001073-06-9 95
Benzene, 1-bromo-2-fluoro- 16035 001072-85-1 93

58 22.15 0.44 C:\DATABASE\NBS75K.L
Benzene, (1-methylethyl)- 3763 000098-82-8 95
Benzene, (1-methylethyl)- 64554 000098-82-8 94
Benzene, (1-methylethyl)- 64556 000098-82-8 94

59 22.49 0.02 C:\DATABASE\NBS75K.L
Benzenethanamine,4-methoxy-.alpha. 67908 023239-32-9 32
Pyridinium, 1-(carboxymethyl)-, hy 6736 024608-93-3 25
Benzenethanamine,4-methoxy-.alpha. 67907 023239-32-9 23

60 22.69 0.07 C:\DATABASE\NBS75K.L
Benzaldehyde 63689 000100-52-7 90
Benzaldehyde 63688 000100-52-7 89
Benzaldehyde 63685 000100-52-7 89

61 22.76 0.23 C:\DATABASE\NBS75K.L
1,4-Cyclohexadiene, 1-methyl-4-(1- 65747 000099-85-4 93
.alpha.-Pinene 65808 000080-56-8 90
.alpha.-Pinene 65809 000080-56-8 87

62 22.97 0.43 C:\DATABASE\NBS75K.L
Benzene, propyl- 64584 000103-65-1 91
Benzene, propyl- 64583 000103-65-1 91
Benzene, propyl- 64582 000103-65-1 90

63 23.12 0.04 C:\DATABASE\NBS75K.L
Bicyclo[2.2.1]heptane, 7,7-dimethy 6625 000471-84-1 92
Bicyclo[2.2.1]heptane, 7,7-dimethy 65761 000471-84-1 55
Bicyclo[2.2.1]heptane, 2,2-dimethy 6695 005794-03-6 52

64 23.19 0.24 C:\DATABASE\NBS75K.L
Camphene 65764 000079-92-5 98
Camphene 65768 000079-92-5 97
Camphene 65766 000079-92-5 97

65 23.37 0.39 C:\DATABASE\NBS75K.L
Benzene, 1,3,5-trimethyl- 64568 000108-67-8 95
Benzene, 1,2,3-trimethyl- 64572 000526-73-8 95
Benzene, 1,2,3-trimethyl- 64573 000526-73-8 95

66 24.12 0.42 C:\DATABASE\NBS75K.L
Benzene, 1,2,4-trimethyl- 64578 000095-63-6 95
Benzene, 1,2,3-trimethyl- 64572 000526-73-8 95
Benzene, 1,2,4-trimethyl- 64577 000095-63-6 95

67 25.00 0.13 C:\DATABASE\NBS75K.L
Benzene, 1-methyl-4-(1-methylethyl 6201 000099-87-6 94
Benzene, methyl(1-methylethyl)- 6208 025155-15-1 93
Benzene, 1-methyl-4-(1-methylethyl 65536 000099-87-6 91

68 25.32 0.17 C:\DATABASE\NBS75K.L
Limonene 6647 000138-86-3 91
Cyclohexene, 1-methyl-4-(1-methyle 65806 005989-54-8 90

D-Limonene 65790 005989-27-5 81

69 25.75 0.03 C:\DATABASE\NBS75K.L
Acetophenone 64533 000098-86-2 70
Acetophenone 64538 000098-86-2 70
Acetophenone 3752 000098-86-2 62

70 25.94 0.04 C:\DATABASE\NBS75K.L
Ethane, 1,1,2-trichloro-1,2,2-trif 69052 000076-13-1 72
Ethane, 1,1,2-trichloro-1,2,2-trif 69050 000076-13-1 50
Ethane, 1,1,2-trichloro-1,2,2-trif 69051 000076-13-1 35

71 26.85 0.06 C:\DATABASE\NBS75K.L
Benzene, methyl(1-methylethenyl)- 65422 026444-18-8 96
Benzene, methyl(1-methylethenyl)- 5892 026444-18-8 95
Benzene, 1-methyl-2-(2-propenyl)- 65419 001587-04-8 94

72 27.39 0.12 C:\DATABASE\NBS75K.L
Butane, 1,1,3,4-tetrachloro-1,2,2, 42990 000423-38-1 43
Butane, 1,2,3,4-tetrachloro-1,1,2, 42989 000375-45-1 43
Ethane, 1,1,2-trichloro-1,2,2-trif 69052 000076-13-1 38

Sun Jun 27 17:01:02 1999

Information from Data File:
File: C:\SARAH\SC3-2.D
Operator:
Date Acquired: 2 Nov 1998 3:59 pm
Method File: TO15D
Sample Name: smog chamber 515 10-29-98
Misc Info:
Vial Number: 1

Search Libraries: C:\DATABASE\NBS75K.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - VOCS.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	0.32	0.05	C:\DATABASE\NBS75K.L			
			Piperidine, 1-nitro-	5328	007119-94-0	4
			2-Nitro-1-propanol	1961	002902-96-7	2
			Ethane	62247	000074-84-0	2
2	0.43	0.05	C:\DATABASE\NBS75K.L			
			Piperidine, 1-nitro-	5328	007119-94-0	4
			Ethane	62248	000074-84-0	2
			Ethane	62247	000074-84-0	2
3	0.84	0.04	C:\DATABASE\NBS75K.L			
			Formaldehyde	10	000050-00-0	1
			Ethane	62246	000074-84-0	1
			Ethane	11	000074-84-0	1
4	2.71	29.92	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	4
			Ethylene oxide	62266	000075-21-8	4
			Acetaldehyde	62265	000075-07-0	3
5	2.94	56.44	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	4
			Ethylene oxide	62266	000075-21-8	4
			Acetaldehyde	62265	000075-07-0	3
6	3.37	3.73	C:\DATABASE\NBS75K.L			
			Dichlorotetrafluoroethane	68163	000076-14-2	62
			Dichlorotetrafluoroethane	14961	000076-14-2	58
			Dichlorodifluoromethane	64510	000075-71-8	27
7	3.61	0.19	C:\DATABASE\NBS75K.L			
			2-Pentanamine	62886	000625-30-9	5
			Carbon dioxide	62263	000124-38-9	4
			Carbon dioxide	34	000124-38-9	4
8	3.72	0.10	C:\DATABASE\NBS75K.L			
			Acetaldehyde	36	000075-07-0	5
			Carbon dioxide	34	000124-38-9	4
			Dextroamphetamine	65628	000051-64-9	4
9	4.77	0.04	C:\DATABASE\NBS75K.L			
			Acetaldehyde	62265	000075-07-0	4
			Acetaldehyde	62264	000075-07-0	4
			Acetaldehyde	36	000075-07-0	4
10	5.28	0.19	C:\DATABASE\NBS75K.L			
			Butane, 2-methyl-	62517	000078-78-4	49
			Butane, 2-methyl-	62518	000078-78-4	47
			Oxirane, 2,2-dimethyl-	62511	000558-30-5	35
11	5.46	0.17	C:\DATABASE\NBS75K.L			
			Acetone	62325	000067-64-1	50
			Acetone	62323	000067-64-1	38
			Acetone	62324	000067-64-1	38

12 5.56 0.27 C:\DATABASE\NBS75K.L
Acetone 62326 000067-64-1 58
Acetone 62324 000067-64-1 53
Acetone 62325 000067-64-1 53

13 6.37 0.09 C:\DATABASE\NBS75K.L
Pentane 280 000109-66-0 38
Pentane 62515 000109-66-0 38
Pentane 62516 000109-66-0 38

14 8.53 0.16 C:\DATABASE\NBS75K.L
Butane, 2,2-dimethyl- 62861 000075-83-2 72
Butane, 2,2-dimethyl- 62862 000075-83-2 64
Butane, 2,2-dimethyl- 732 000075-83-2 64

15 9.76 0.05 C:\DATABASE\NBS75K.L
2-Oxetanone, 4,4-dimethyl- 1450 001823-52-5 32
1-Pentene, 4-methyl- 599 000691-37-2 27
4-Pentenal 571 002100-17-6 12

16 10.02 0.09 C:\DATABASE\NBS75K.L
1-Pentene 62464 000109-67-1 72
Cyclopentane 234 000287-92-3 72
1-Pentene 62466 000109-67-1 64

17 10.19 0.13 C:\DATABASE\NBS75K.L
Butane, 2,3-dimethyl- 62870 000079-29-8 80
Butane, 2,3-dimethyl- 62869 000079-29-8 72
Butane, 2,3-dimethyl- 735 000079-29-8 50

18 10.46 0.12 C:\DATABASE\NBS75K.L
Pentane, 2-methyl- 733 000107-83-5 74
Pentane, 2-methyl- 62865 000107-83-5 72
Pentane, 2-methyl- 62863 000107-83-5 72

19 10.57 0.03 C:\DATABASE\NBS75K.L
1-Butene, 2-methyl- 62458 000563-46-2 43
Cyclopropane, 1,1-dimethyl- 62468 001630-94-0 43
1-Butene, 3-methyl- 236 000563-45-1 38

20 10.79 0.08 C:\DATABASE\NBS75K.L
Butanal 62486 000123-72-8 91
Butanal 265 000123-72-8 90
Butanal 62487 000123-72-8 90

21 11.12 0.06 C:\DATABASE\NBS75K.L
2-Butanone 62493 000078-93-3 53
2-Butanone 266 000078-93-3 40
2-Butanone 62492 000078-93-3 9

22 11.16 0.14 C:\DATABASE\NBS75K.L
Pentane, 3-methyl- 734 000096-14-0 43
Heptane, 2,2,4-trimethyl- 8105 014720-74-2 40
Pentane, 3-methyl- 62867 000096-14-0 38

23 12.02 0.13 C:\DATABASE\NBS75K.L
Hexane 62874 000110-54-3 64
Hexane 62873 000110-54-3 50
Hexane 736 000110-54-3 49

24 13.14 0.12 C:\DATABASE\NBS75K.L
Cyclopentane, methyl- 594 000096-37-7 83
Cyclopentane, methyl- 62763 000096-37-7 64
Cyclobutane, ethyl- 604 004806-61-5 59

25 13.37 0.17 C:\DATABASE\NBS75K.L
Pentane, 2,4-dimethyl- 63424 000108-08-7 80
Pentane, 2,4-dimethyl- 63425 000108-08-7 64
Pentane, 2,4-dimethyl- 1594 000108-08-7 47

26 13.65 0.03 C:\DATABASE\NBS75K.L
2-Butanamine 62535 013952-84-6 9
Ethylene oxide 62267 000075-21-8 4
n-Hexylmethylamine 3165 035161-70-7 4

27 13.96 0.03 C:\DATABASE\NBS75K.L
2-Pentanone 62837 000107-87-9 10
2-Butanone, 3-methyl- 703 000563-80-4 10
2-Pentanone 62835 000107-87-9 9

28 14.14 0.25 C:\DATABASE\NBS75K.L
Benzene 62628 000071-43-2 91
Benzene 62627 000071-43-2 91
Benzene 62626 000071-43-2 91

29 14.48 0.17 C:\DATABASE\NBS75K.L
Cyclohexane 62777 000110-82-7 93
Cyclohexane 62778 000110-82-7 81
Cyclohexane 62776 000110-82-7 76

30 14.86 0.24 C:\DATABASE\NBS75K.L
Hexane, 2-methyl- 1598 000591-76-4 64
Hexane, 2-methyl- 63434 000591-76-4 64
Hexane, 2-methyl- 63435 000591-76-4 62

31 14.92 0.32 C:\DATABASE\NBS75K.L
Pentane, 2,3-dimethyl- 63429 000565-59-3 52
Pentane, 2,3-dimethyl- 63431 000565-59-3 52
Pentane, 2,3-dimethyl- 63430 000565-59-3 49

32 15.17 0.25 C:\DATABASE\NBS75K.L
Hexane, 3-methyl- 63422 000589-34-4 74
Hexane, 3-methyl- 63421 000589-34-4 72
Hexane, 3-methyl- 63423 000589-34-4 64

33 15.65 0.38 C:\DATABASE\NBS75K.L
Pentane, 2,2,4-trimethyl- 64220 000540-84-1 78
Heptane, 2,2,4,6,6-pentamethyl- 68260 013475-82-6 78
Hexane, 2,2-dimethyl- 64216 000590-73-8 78

34 15.93 1.41 C:\DATABASE\NBS75K.L
Benzene, methyl-, trifluoro deriv. 8769 027359-10-0 96
Benzene, (trifluoromethyl)- 8768 000098-08-8 95
Benzene, (trifluoromethyl)- 66428 000098-08-8 94

35 16.02 0.19 C:\DATABASE\NBS75K.L
Heptane 63440 000142-82-5 93
Heptane 63438 000142-82-5 90
Heptane 1600 000142-82-5 72

36 16.37 0.05 C:\DATABASE\NBS75K.L
1-Pentene, 2,4,4-trimethyl- 64024 000107-39-1 25
1-Pentene, 2,4,4-trimethyl- 64025 000107-39-1 14
2-Hexene, 5,5-dimethyl-, (Z)- 64046 039761-61-0 14

37 16.71 0.19 C:\DATABASE\NBS75K.L
Cyclohexane, methyl- 1326 000108-87-2 93
Cyclohexane, methyl- 63236 000108-87-2 81
Cyclohexane, methyl- 63235 000108-87-2 81

38 17.63 0.28 C:\DATABASE\NBS75K.L
Pentane, 2,3,4-trimethyl- 3100 000565-75-3 83
Heptane, 4-methyl- 3096 000589-53-7 78
Pentane, 2,3,4-trimethyl- 64228 000565-75-3 74

39 17.77 0.28 C:\DATABASE\NBS75K.L
Toluene 63028 000108-88-3 95
Toluene 965 000108-88-3 93
Toluene 63029 000108-88-3 90

40 18.07 0.29 C:\DATABASE\NBS75K.L

Heptane, 2-methyl- 3092 000592-27-8 87
Heptane, 2-methyl- 64218 000592-27-8 81
1-Propanol, 2,2-dimethyl-, propano 8370 003581-69-9 72

41 18.29 0.25 C:\DATABASE\NBS75K.L
Octane, 3,4-dimethyl- 8107 015869-92-8 64
Heptane, 3-methyl- 64227 000589-81-1 58
Heptane, 4-ethyl- 5148 002216-32-2 53

42 18.42 0.03 C:\DATABASE\NBS75K.L
Hexanal 63408 000066-25-1 38
Hexanal 63409 000066-25-1 32
Hexanal 63410 000066-25-1 25

43 18.99 0.25 C:\DATABASE\NBS75K.L
Octane 64209 000111-65-9 87
Octane 64207 000111-65-9 76
Octane 3084 000111-65-9 74

44 20.41 0.28 C:\DATABASE\NBS75K.L
Ethylbenzene 63690 000100-41-4 93
Ethylbenzene 2026 000100-41-4 93
Ethylbenzene 63691 000100-41-4 87

45 20.66 0.33 C:\DATABASE\NBS75K.L
Benzene, 1,2-dimethyl- 63705 000095-47-6 94
Benzene, 1,2-dimethyl- 63706 000095-47-6 94
Benzene, 1,3-dimethyl- 63695 000108-38-3 94

46 21.14 0.03 C:\DATABASE\NBS75K.L
L-Alanine, methyl ester 63591 010065-72-2 36
Phenylpropanolamine 66860 000492-41-1 36
Amphetamine-3-methyl 9506 000000-00-0 36

47 21.28 0.21 C:\DATABASE\NBS75K.L
Benzene, 1,3-dimethyl- 63695 000108-38-3 95
Benzene, 1,2-dimethyl- 63706 000095-47-6 94
p-Xylene 63700 000106-42-3 94

48 21.64 0.25 C:\DATABASE\NBS75K.L
Nonane 65142 000111-84-2 76
Undecane 67317 001120-21-4 59
Octane 3084 000111-65-9 50

49 21.93 0.26 C:\DATABASE\NBS75K.L
Benzene, 1-bromo-3-fluoro- 16034 001073-06-9 95
Benzene, 1-bromo-2-fluoro- 16035 001072-85-1 94
Benzene, 1-bromo-3-fluoro- 68407 001073-06-9 93

50 22.15 0.33 C:\DATABASE\NBS75K.L
Benzene, (1-methylethyl)- 3763 000098-82-8 94
Benzene, (1-methylethyl)- 64554 000098-82-8 93
Benzene, (1-methylethyl)- 64553 000098-82-8 93

51 22.71 0.20 C:\DATABASE\NBS75K.L
Benzaldehyde 63688 000100-52-7 96
Benzaldehyde 63689 000100-52-7 96
Benzaldehyde 2020 000100-52-7 93

52 22.98 0.28 C:\DATABASE\NBS75K.L
Benzene, propyl- 64583 000103-65-1 91
Benzene, propyl- 3781 000103-65-1 90
Benzene, propyl- 64582 000103-65-1 90

53 23.38 0.03 C:\DATABASE\NBS75K.L
1,2,4-Trimethylbenzene 3771 000095-36-3 86
Benzene, 1,3,5-trimethyl- 64570 000108-67-8 86
Benzene, 1,2,3-trimethyl- 64576 000526-73-8 86

54 24.13 0.11 C:\DATABASE\NBS75K.L
Benzene, 1,2,3-trimethyl- 64576 000526-73-8 95

Benzene, 1,3,5-trimethyl- 64570 000108-67-8 94
1,2,4-Trimethylbenzene 3771 000095-36-3 93

55 25.77 0.05 C:\DATABASE\NBS75K.L
Acetophenone 64538 000098-86-2 81
Acetophenone 64534 000098-86-2 81
Acetophenone 64533 000098-86-2 81

56 25.95 0.05 C:\DATABASE\NBS75K.L
Ethane, 1,1,2-trichloro-1,2,2-trif 69052 000076-13-1 53
Ethane, 1,1,2-trichloro-1,2,2-trif 69051 000076-13-1 40
Ethane, 1,1,2-trichloro-1,2,2-trif 69050 000076-13-1 40

57 27.39 0.12 C:\DATABASE\NBS75K.L
Butane, 1,1,3,4-tetrachloro-1,2,2, 42990 000423-38-1 72
Ethane, 1,1,2-trichloro-1,2,2-trif 69051 000076-13-1 38
Ethane, 1,1,2-trichloro-1,2,2-trif 69052 000076-13-1 38

Sun Jun 27 17:02:55 1999

Information from Data File:
File: C:\SARAH\SC6-1.D
Operator:
Date Acquired: 15 Apr 1999 7:23 pm
Method File: TO15D
Sample Name:
Misc Info: 1000cc
Vial Number: 1

Search Libraries: C:\DATABASE\NBS75K.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - VOCS.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	0.14	0.06	C:\DATABASE\NBS75K.L			
			Ethane	62248	000074-84-0	2
			Ethane	62247	000074-84-0	2
			Ethane	11	000074-84-0	2
2	0.18	0.04	C:\DATABASE\NBS75K.L			
			Ethane	62248	000074-84-0	2
			Ethane	62247	000074-84-0	2
			Formaldehyde	10	000050-00-0	2
3	0.39	0.38	C:\DATABASE\NBS75K.L			
			Ethane	62248	000074-84-0	2
			Ethane	62247	000074-84-0	2
			Ethane	62246	000074-84-0	2
4	0.46	0.07	C:\DATABASE\NBS75K.L			
			Ethane	62248	000074-84-0	2
			Ethane	62247	000074-84-0	2
			Ethane	11	000074-84-0	2
5	0.52	0.05	C:\DATABASE\NBS75K.L			
			Ethane	62248	000074-84-0	2
			Ethane	62247	000074-84-0	2
			Ethane	62246	000074-84-0	1
6	2.65	18.90	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	4
			Ethylene oxide	62266	000075-21-8	4
			Acetaldehyde	62265	000075-07-0	3
7	2.71	6.31	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	3
			Carbon dioxide	34	000124-38-9	3
			Carbon dioxide	62263	000124-38-9	3
8	2.87	61.30	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	4
			Ethylene oxide	62266	000075-21-8	4
			Acetaldehyde	62265	000075-07-0	3
9	3.30	2.93	C:\DATABASE\NBS75K.L			
			Dichlorotetrafluoroethane	68163	000076-14-2	62
			Dichlorotetrafluoroethane	14961	000076-14-2	52
			Dichlorodifluoromethane	3658	000075-71-8	25
10	3.53	0.26	C:\DATABASE\NBS75K.L			
			Carbon dioxide	62263	000124-38-9	4
			Carbon dioxide	34	000124-38-9	4
			Benzeneethanamine, N-methyl-	6311	000589-08-2	4
11	3.64	0.10	C:\DATABASE\NBS75K.L			
			Butane	62336	000106-97-8	9
			Butane	99	000106-97-8	9
			Carbon dioxide	34	000124-38-9	4

12 3.78 0.12 C:\DATABASE\NBS75K.L
Carbon dioxide 34 000124-38-9 4
Carbon dioxide 62263 000124-38-9 4
2-Propenal 72 000107-02-8 4

13 4.00 0.10 C:\DATABASE\NBS75K.L
2-Propenal 72 000107-02-8 5
Carbon dioxide 62263 000124-38-9 4
Carbon dioxide 34 000124-38-9 4

14 4.66 0.11 C:\DATABASE\NBS75K.L
1-Butene, 2-methyl- 62457 000563-46-2 45
1-Butene, 3-methyl- 236 000563-45-1 45
2-Butene, 2-methyl- 62462 000513-35-9 43

15 5.16 0.20 C:\DATABASE\NBS75K.L
Butane, 2-methyl- 62517 000078-78-4 49
Butane, 2-methyl- 62518 000078-78-4 49
Butane, 2-methyl- 281 000078-78-4 43

16 5.30 0.12 C:\DATABASE\NBS75K.L
Acetone 62325 000067-64-1 43
Acetone 62326 000067-64-1 37
Acetone 62322 000067-64-1 37

17 5.35 0.18 C:\DATABASE\NBS75K.L
Acetone 62326 000067-64-1 58
Acetone 62325 000067-64-1 53
Acetone 62323 000067-64-1 42

18 5.70 0.10 C:\DATABASE\NBS75K.L
Cyclopropane, ethyl- 227 001191-96-4 60
1-Pentene 62464 000109-67-1 53
1-Pentene 230 000109-67-1 49

19 6.21 0.09 C:\DATABASE\NBS75K.L
Pentane 62516 000109-66-0 38
Pentane 62515 000109-66-0 38
Pentane 280 000109-66-0 38

20 6.46 0.06 C:\DATABASE\NBS75K.L
1,3-Butadiene, 2-methyl- 184 000078-79-5 81
1-Butyne, 3-methyl- 186 000598-23-2 38
1,3-Pentadiene, (Z)- 176 001574-41-0 30

21 6.67 0.08 C:\DATABASE\NBS75K.L
Cyclopropane, 1,2-dimethyl-, cis- 62467 000930-18-7 46
1-Butene, 3-methyl- 236 000563-45-1 45
2-Pentene 231 000109-68-2 43

22 7.17 0.08 C:\DATABASE\NBS75K.L
2-Pentene, (Z)- 62456 000627-20-3 70
2-Pentene, (E)- 233 000646-04-8 58
2-Pentene, (Z)- 224 000627-20-3 58

23 7.48 0.06 C:\DATABASE\NBS75K.L
2-Butene, 2-methyl- 62462 000513-35-9 58
1-Butene, 3-methyl- 236 000563-45-1 52
2-Pentene 231 000109-68-2 52

24 8.37 0.14 C:\DATABASE\NBS75K.L
Butane, 2,2-dimethyl- 62862 000075-83-2 64
Butane, 2,2-dimethyl- 732 000075-83-2 64
Butane, 2,2-dimethyl- 62861 000075-83-2 64

25 9.31 0.10 C:\DATABASE\NBS75K.L
Cyclopentene 62412 000142-29-0 87
Cyclopentene 185 000142-29-0 87
Cyclopentene 62411 000142-29-0 87

26 9.62 0.13 C:\DATABASE\NBS75K.L
1-Pentene, 4-methyl- 599 000691-37-2 52
1-Propene, 2-methyl- 62305 000115-11-7 46
1-Propene, 2-methyl- 62306 000115-11-7 46

27 9.89 0.10 C:\DATABASE\NBS75K.L
Cyclobutane, methyl- 229 000598-61-8 72
Cyclopentane 234 000287-92-3 64
Cyclopropane, ethyl- 227 001191-96-4 64

28 10.07 0.14 C:\DATABASE\NBS75K.L
Butane, 2,3-dimethyl- 62871 000079-29-8 80
Butane, 2,3-dimethyl- 62870 000079-29-8 80
Butane, 2,3-dimethyl- 62869 000079-29-8 64

29 10.34 0.16 C:\DATABASE\NBS75K.L
Pentane, 2-methyl- 733 000107-83-5 87
Pentane, 2-methyl- 62863 000107-83-5 83
Pentane, 2-methyl- 62865 000107-83-5 80

30 11.05 0.15 C:\DATABASE\NBS75K.L
Pentane, 3-methyl- 734 000096-14-0 80
Pentane, 3-methyl- 62868 000096-14-0 80
Pentane, 3-methyl- 62867 000096-14-0 80

31 11.32 0.10 C:\DATABASE\NBS75K.L
1-Pentene, 2-methyl- 598 000763-29-1 93
1-Pentene, 2-methyl- 62768 000763-29-1 93
1-Hexene, 3,4-dimethyl- 2717 016745-94-1 47

32 11.92 0.16 C:\DATABASE\NBS75K.L
Hexane 62874 000110-54-3 64
Hexane 736 000110-54-3 58
Hexane 62873 000110-54-3 53

33 12.16 0.13 C:\DATABASE\NBS75K.L
2-Hexene 589 000592-43-8 94
2-Hexene, (E)- 62751 004050-45-7 93
2-Hexene, (E)- 62752 004050-45-7 87

34 12.56 0.13 C:\DATABASE\NBS75K.L
2-Hexene 589 000592-43-8 94
2-Hexene, (E)- 62752 004050-45-7 76
2-Hexene, (E)- 62751 004050-45-7 76

35 13.03 0.15 C:\DATABASE\NBS75K.L
Cyclopentane, methyl- 594 000096-37-7 87
Cyclopentane, methyl- 62763 000096-37-7 72
1H-Tetrazole, 5-methyl- 529 004076-36-2 64

36 13.26 0.19 C:\DATABASE\NBS75K.L
Pentane, 2,4-dimethyl- 1594 000108-08-7 87
Pentane, 2,4-dimethyl- 63424 000108-08-7 58
Pentane, 2,4-dimethyl- 63425 000108-08-7 56

37 14.02 0.13 C:\DATABASE\NBS75K.L
Benzene 62628 000071-43-2 93
Benzene 62627 000071-43-2 90
Benzene 62626 000071-43-2 90

38 14.37 0.20 C:\DATABASE\NBS75K.L
Cyclohexane 62777 000110-82-7 93
Cyclohexane 606 000110-82-7 87
Cyclohexane 62779 000110-82-7 87

39 14.76 0.26 C:\DATABASE\NBS75K.L
Hexane, 2-methyl- 1598 000591-76-4 83
Hexane, 2-methyl- 63435 000591-76-4 81
Hexane, 2-methyl- 63433 000591-76-4 80

40 14.81 0.23 C:\DATABASE\NBS75K.L

Pentane, 2,3-dimethyl- 1597 000565-59-3 90
Pentane, 2,3-dimethyl- 63429 000565-59-3 90
Pentane, 2,3-dimethyl- 63431 000565-59-3 90

41 15.07 0.25 C:\DATABASE\NBS75K.L
Hexane, 3-methyl- 63423 000589-34-4 93
Hexane, 3-methyl- 1593 000589-34-4 87
Hexane, 3-methyl- 63421 000589-34-4 87

42 15.45 0.07 C:\DATABASE\NBS75K.L
Trichloroethylene 65175 000079-01-6 95
Trichloroethylene 65176 000079-01-6 93
Trichloroethylene 5300 000079-01-6 49

43 15.54 0.34 C:\DATABASE\NBS75K.L
Hexane, 2,2-dimethyl- 64217 000590-73-8 64
Butane, 2,2,3,3-tetramethyl- 64215 000594-82-1 64
Pentane, 2,2,4-trimethyl- 64220 000540-84-1 59

44 15.82 0.63 C:\DATABASE\NBS75K.L
Benzene, (trifluoromethyl)- 66428 000098-08-8 97
Benzene, methyl-, trifluoro deriv. 8769 027359-10-0 96
Benzene, (trifluoromethyl)- 8768 000098-08-8 96

45 15.91 0.25 C:\DATABASE\NBS75K.L
Heptane 63440 000142-82-5 93
Heptane 63438 000142-82-5 90
Heptane 1600 000142-82-5 87

46 16.61 0.26 C:\DATABASE\NBS75K.L
Cyclohexane, methyl- 1326 000108-87-2 96
Cyclohexane, methyl- 63236 000108-87-2 96
Cyclohexane, methyl- 63235 000108-87-2 93

47 17.53 0.32 C:\DATABASE\NBS75K.L
Pentane, 2,3,4-trimethyl- 3100 000565-75-3 91
Pentane, 2,3,4-trimethyl- 64228 000565-75-3 86
Pentane, 3-ethyl- 1595 000617-78-7 78

48 17.67 0.26 C:\DATABASE\NBS75K.L
Toluene 63029 000108-88-3 93
Toluene 965 000108-88-3 93
Toluene 63030 000108-88-3 90

49 17.97 0.35 C:\DATABASE\NBS75K.L
Heptane, 2-methyl- 3092 000592-27-8 91
Heptane, 2-methyl- 64218 000592-27-8 87
Hexane, 2,5-dimethyl- 64206 000592-13-2 72

50 18.19 0.33 C:\DATABASE\NBS75K.L
Heptane, 3-methyl- 3099 000589-81-1 90
Heptane, 3-methyl- 64227 000589-81-1 74
Hexane, 1-(hexyloxy)-2-methyl- 23019 074421-17-3 64

51 18.90 0.34 C:\DATABASE\NBS75K.L
Octane 64209 000111-65-9 93
Octane 3084 000111-65-9 90
Octane 64207 000111-65-9 90

52 20.31 0.30 C:\DATABASE\NBS75K.L
Ethylbenzene 63690 000100-41-4 93
Ethylbenzene 2026 000100-41-4 93
Ethylbenzene 63692 000100-41-4 93

53 20.55 0.53 C:\DATABASE\NBS75K.L
Benzene, 1,3-dimethyl- 63695 000108-38-3 94
Benzene, 1,2-dimethyl- 63706 000095-47-6 94
Benzene, 1,2-dimethyl- 63707 000095-47-6 94

54 21.17 0.27 C:\DATABASE\NBS75K.L
Benzene, 1,3-dimethyl- 63697 000108-38-3 94

Benzene, 1,2-dimethyl- 63705 000095-47-6 94
Benzene, 1,2-dimethyl- 63706 000095-47-6 94

55 21.54 0.40 C:\DATABASE\NBS75K.L
Nonane 65145 000111-84-2 93
Nonane 65142 000111-84-2 90
Nonane 65144 000111-84-2 81

56 22.04 0.28 C:\DATABASE\NBS75K.L
Benzene, (1-methylethyl)- 3763 000098-82-8 93
Benzene, (1-methylethyl)- 64552 000098-82-8 90
Benzene, (1-methylethyl)- 64553 000098-82-8 90

57 22.86 0.29 C:\DATABASE\NBS75K.L
Benzene, propyl- 64584 000103-65-1 94
Benzene, propyl- 64583 000103-65-1 91
Benzene, propyl- 3781 000103-65-1 90

58 24.01 0.08 C:\DATABASE\NBS75K.L
Benzene, 1,2,3-trimethyl- 64572 000526-73-8 94
Benzene, 1,2,3-trimethyl- 64573 000526-73-8 93
1,2,4-Trimethylbenzene 3771 000095-36-3 90

59 27.26 0.10 C:\DATABASE\NBS75K.L
Butane, 1,1,3,4-tetrachloro-1,2,2, 42990 000423-38-1 50
Ethane, 1,1,2-trichloro-1,2,2-trif 69052 000076-13-1 43
Ethane, 1,1,2-trichloro-1,2,2-trif 69050 000076-13-1 13

Sun Jun 27 17:05:09 1999

Information from Data File:
File: C:\SARAH\SC6-2.D
Operator:
Date Acquired: 15 Apr 1999 8:33 pm
Method File: TO15D
Sample Name:
Misc Info: 1000cc
Vial Number: 1

Search Libraries: C:\DATABASE\NBS75K.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - VOCS.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	0.16	0.10	C:\DATABASE\NBS75K.L			
			Ethane	62248	000074-84-0	2
			Ethane	62247	000074-84-0	2
			Ethane	62246	000074-84-0	2
2	0.37	0.06	C:\DATABASE\NBS75K.L			
			Ethane	62248	000074-84-0	2
			Ethane	62247	000074-84-0	2
			Ethane	11	000074-84-0	2
3	0.41	0.07	C:\DATABASE\NBS75K.L			
			Ethane	62248	000074-84-0	2
			Ethane	62247	000074-84-0	2
			Ethane	11	000074-84-0	2
4	0.48	0.04	C:\DATABASE\NBS75K.L			
			Ethane	62248	000074-84-0	2
			Ethane	62247	000074-84-0	2
			Ethane	62246	000074-84-0	1
5	2.65	21.69	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	4
			Ethylene oxide	62266	000075-21-8	4
			Acetaldehyde	62265	000075-07-0	3
6	2.72	1.21	C:\DATABASE\NBS75K.L			
			Acetaldehyde	62264	000075-07-0	2
			Acetaldehyde	36	000075-07-0	2
			Carbon dioxide	34	000124-38-9	2
7	2.79	10.77	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	3
			Carbon dioxide	34	000124-38-9	3
			Carbon dioxide	62263	000124-38-9	3
8	2.89	54.34	C:\DATABASE\NBS75K.L			
			Ethylene oxide	62267	000075-21-8	4
			Ethylene oxide	62266	000075-21-8	4
			Acetaldehyde	62265	000075-07-0	3
9	3.30	3.35	C:\DATABASE\NBS75K.L			
			Dichlorotetrafluoroethane	68163	000076-14-2	62
			Dichlorotetrafluoroethane	14961	000076-14-2	52
			Dichlorodifluoromethane	64510	000075-71-8	35
10	3.53	0.29	C:\DATABASE\NBS75K.L			
			Carbon dioxide	34	000124-38-9	4
			Carbon dioxide	62263	000124-38-9	4
			Acetaldehyde	36	000075-07-0	4
11	3.64	0.31	C:\DATABASE\NBS75K.L			
			Acetaldehyde	62264	000075-07-0	5
			Ethylene oxide	62267	000075-21-8	4
			Acetaldehyde	36	000075-07-0	4

12 3.78 0.06 C:\DATABASE\NBS75K.L
Acetaldehyde 36 000075-07-0 5
Carbon dioxide 62263 000124-38-9 4
Carbon dioxide 34 000124-38-9 4

13 4.66 0.06 C:\DATABASE\NBS75K.L
1-Butene, 3-methyl- 236 000563-45-1 25
2-Butene, 2-methyl- 62462 000513-35-9 22
1-Butene, 2-methyl- 62457 000563-46-2 22

14 5.16 0.19 C:\DATABASE\NBS75K.L
Butane, 2-methyl- 62518 000078-78-4 49
Butane, 2-methyl- 62517 000078-78-4 49
Butane, 2-methyl- 281 000078-78-4 43

15 5.30 0.07 C:\DATABASE\NBS75K.L
Acetone 62325 000067-64-1 38
Acetone 62324 000067-64-1 38
2-Pentanamine 62886 000625-30-9 12

16 5.34 0.16 C:\DATABASE\NBS75K.L
Acetone 62325 000067-64-1 43
Acetone 62326 000067-64-1 43
Acetone 94 000067-64-1 32

17 5.44 0.21 C:\DATABASE\NBS75K.L
Acetone 62326 000067-64-1 52
Acetone 62325 000067-64-1 50
Acetone 62324 000067-64-1 50

18 5.70 0.05 C:\DATABASE\NBS75K.L
Carbon dioxide 62263 000124-38-9 3
Carbon dioxide 34 000124-38-9 3
Acetaldehyde 36 000075-07-0 3

19 6.21 0.11 C:\DATABASE\NBS75K.L
Pentane 280 000109-66-0 43
Pentane 62515 000109-66-0 38
Pentane 62516 000109-66-0 38

20 8.38 0.14 C:\DATABASE\NBS75K.L
Butane, 2,2-dimethyl- 62862 000075-83-2 64
Butane, 2,2-dimethyl- 732 000075-83-2 59
Butane, 2,2-dimethyl- 62861 000075-83-2 53

21 9.62 0.08 C:\DATABASE\NBS75K.L
Furan, 2,3-dihydro- 62438 001191-99-7 43
1-Pentene, 4-methyl- 599 000691-37-2 38
1-Propene, 2-methyl- 62305 000115-11-7 38

22 9.88 0.09 C:\DATABASE\NBS75K.L
Cyclopentane 234 000287-92-3 72
1-Pentene 62464 000109-67-1 72
Cyclobutane, methyl- 229 000598-61-8 64

23 10.06 0.13 C:\DATABASE\NBS75K.L
Butane, 2,3-dimethyl- 62870 000079-29-8 72
Butane, 2,3-dimethyl- 735 000079-29-8 64
cis-1,3-Cyclohexanediamine 2958 026772-34-9 43

24 10.33 0.13 C:\DATABASE\NBS75K.L
Pentane, 2-methyl- 733 000107-83-5 87
Pentane, 2-methyl- 62863 000107-83-5 83
Pentane, 2-methyl- 62864 000107-83-5 72

25 11.04 0.16 C:\DATABASE\NBS75K.L
Pentane, 3-methyl- 62867 000096-14-0 74
Pentane, 3-methyl- 734 000096-14-0 72
Pentane, 3-methyl- 62868 000096-14-0 72

26 11.91 0.15 C:\DATABASE\NBS75K.L
Hexane 62874 000110-54-3 59
Hexane 62873 000110-54-3 50
Hexane 736 000110-54-3 49

27 13.03 0.13 C:\DATABASE\NBS75K.L
Cyclopentane, methyl- 594 000096-37-7 76
Cyclopentane, methyl- 62763 000096-37-7 64
Cyclobutane, ethyl- 604 004806-61-5 50

28 13.27 0.17 C:\DATABASE\NBS75K.L
Pentane, 2,4-dimethyl- 63424 000108-08-7 87
Pentane, 2,4-dimethyl- 1594 000108-08-7 74
Pentane, 2,4-dimethyl- 63425 000108-08-7 52

29 14.03 0.14 C:\DATABASE\NBS75K.L
Benzene 62628 000071-43-2 93
1,3-Hexadien-5-yne 404 010420-90-3 91
Benzene 62627 000071-43-2 90

30 14.37 0.17 C:\DATABASE\NBS75K.L
Cyclohexane 62776 000110-82-7 81
Cyclohexane 62778 000110-82-7 81
Cyclohexane 606 000110-82-7 81

31 14.76 0.23 C:\DATABASE\NBS75K.L
Hexane, 2-methyl- 1598 000591-76-4 87
Hexane, 2-methyl- 63435 000591-76-4 81
Hexane, 2-methyl- 63433 000591-76-4 80

32 14.82 0.25 C:\DATABASE\NBS75K.L
Pentane, 2,3-dimethyl- 63430 000565-59-3 87
Pentane, 2,3-dimethyl- 63431 000565-59-3 87
Pentane, 2,3-dimethyl- 63429 000565-59-3 87

33 15.07 0.22 C:\DATABASE\NBS75K.L
Hexane, 3-methyl- 63423 000589-34-4 93
Hexane, 3-methyl- 1593 000589-34-4 87
Hexane, 3-methyl- 63421 000589-34-4 86

34 15.45 0.08 C:\DATABASE\NBS75K.L
Trichloroethylene 5300 000079-01-6 93
Trichloroethylene 65175 000079-01-6 93
Trichloroethylene 65176 000079-01-6 86

35 15.54 0.33 C:\DATABASE\NBS75K.L
Butane, 2,2,3,3-tetramethyl- 3090 000594-82-1 53
Hexane, 2,2,5-trimethyl- 65128 003522-94-9 53
Hexane, 2,2,4-trimethyl- 65103 016747-26-5 53

36 15.83 0.62 C:\DATABASE\NBS75K.L
Benzene, methyl-, trifluoro deriv. 8769 027359-10-0 96
Benzene, (trifluoromethyl)- 66428 000098-08-8 95
Benzene, (trifluoromethyl)- 8768 000098-08-8 93

37 15.92 0.22 C:\DATABASE\NBS75K.L
Heptane 63440 000142-82-5 93
Heptane 63438 000142-82-5 90
Heptane 1600 000142-82-5 87

38 16.60 0.21 C:\DATABASE\NBS75K.L
Cyclohexane, methyl- 63236 000108-87-2 96
Cyclohexane, methyl- 1326 000108-87-2 96
Cyclohexane, methyl- 63235 000108-87-2 93

39 17.53 0.28 C:\DATABASE\NBS75K.L
Pentane, 2,3,4-trimethyl- 3100 000565-75-3 91
Pentane, 2,3,4-trimethyl- 64228 000565-75-3 91
Pentane, 2,3,4-trimethyl- 64229 000565-75-3 78

40 17.67 0.23 C:\DATABASE\NBS75K.L

Toluene 965 000108-88-3 93
Toluene 63029 000108-88-3 93
Toluene 63030 000108-88-3 90

41 17.97 0.29 C:\DATABASE\NBS75K.L
Heptane, 2-methyl- 3092 000592-27-8 90
Heptane, 2-methyl- 64218 000592-27-8 81
Hexane, 2,5-dimethyl- 64205 000592-13-2 59

42 18.19 0.28 C:\DATABASE\NBS75K.L
Heptane, 3-methyl- 64227 000589-81-1 87
Heptane, 3-methyl- 3099 000589-81-1 72
Hexane, 1-(hexyloxy)-2-methyl- 23019 074421-17-3 59

43 18.90 0.29 C:\DATABASE\NBS75K.L
Octane 64209 000111-65-9 93
Octane 3084 000111-65-9 83
Octane 64207 000111-65-9 74

44 20.30 0.26 C:\DATABASE\NBS75K.L
Ethylbenzene 63692 000100-41-4 93
Ethylbenzene 2026 000100-41-4 93
Ethylbenzene 63690 000100-41-4 93

45 20.55 0.38 C:\DATABASE\NBS75K.L
p-Xylene 63699 000106-42-3 95
p-Xylene 63702 000106-42-3 95
Benzene, 1,3-dimethyl- 63695 000108-38-3 95

46 21.17 0.21 C:\DATABASE\NBS75K.L
Benzene, 1,2-dimethyl- 63705 000095-47-6 94
Benzene, 1,2-dimethyl- 63706 000095-47-6 94
p-Xylene 63702 000106-42-3 94

47 21.53 0.32 C:\DATABASE\NBS75K.L
Nonane 65144 000111-84-2 94
Nonane 65142 000111-84-2 90
Nonane 65145 000111-84-2 81

48 22.04 0.28 C:\DATABASE\NBS75K.L
Benzene, (1-methylethyl)- 3763 000098-82-8 93
Benzene, (1-methylethyl)- 64556 000098-82-8 90
Benzene, (1-methylethyl)- 64553 000098-82-8 90

49 22.86 0.28 C:\DATABASE\NBS75K.L
Benzene, propyl- 64583 000103-65-1 91
Benzene, propyl- 64582 000103-65-1 90
Benzene, propyl- 3781 000103-65-1 90

50 23.25 0.04 C:\DATABASE\NBS75K.L
Benzene, 1,3,5-trimethyl- 64570 000108-67-8 92
Benzene, 1,2,4-trimethyl- 3775 000095-63-6 64
Benzene, 1,2,4-trimethyl- 64578 000095-63-6 64

51 24.01 0.10 C:\DATABASE\NBS75K.L
1,2,4-Trimethylbenzene 3771 000095-36-3 95
Benzene, 1,3,5-trimethyl- 64570 000108-67-8 95
Benzene, 1,2,3-trimethyl- 64572 000526-73-8 94

Sun Jun 27 17:07:04 1999

Appendix C

FID Analysis

0.682		ISTD 1	7.877
Smog Chamber		ISTD 2	16.967
c:\sarah\1-1		ISTD 3	22.62
c:\ezchrom\methods\0to15.met			
Syste m			
Peaks	55		

RT (min)	Peak ID	Compound	Area	Height	Area of Knowns	Area of Unknowns	Conc (ppbv)	ppbC
6.557	5	propane	18461	6028	18461	-	2.7	8.1
6.637	?	?	13696	4445	-	13696	-	-
7.877	9	ISTD 1	169784	49311	-	-	-	-
8.317	11b	1,3-butadiene	12309	3236	12309	-	0.7	2.9
8.477	?	?	27669	8686	-	27669	-	-
8.71	?	?	21992	7690	-	21992	-	-
9.01	?	?	22150	8013	-	22150	-	-
9.413	?	?	18073	6653	-	18073	-	-
10.35	19	ethanol	26831	10000	26831	-	11.5	22.9
10.5	?	?	9345	1696	-	9345	-	-
10.7	20b	2-propenal	12609	4287	12609	-	3.9	11.8
10.88	21	isopentane	47728	18352	47728	-	4.5	22.6
10.96	22b	acetone/propanal	112505	29247	112505	-	47.0	141.1
11.33	?	?	25651	9865	-	25651	-	-
11.67	?	?	23441	9503	-	23441	-	-
11.81	24	n-pentane	16045	6397	16045	-	1.4	6.8
11.91	25	isoprene	22493	9376	22493	-	2.2	11.2
12.13	26b	1,1-dichloroethylene	22593	9026	22593	-	4.6	9.3
12.27	27	cis-2-pentene	13682	5510	13682	-	1.0	5.2
12.71	?	?	29142	11180	-	29142	-	-
13.21	?	?	25366	8548	-	25366	-	-
13.31	?	?	32491	11983	-	32491	-	-
13.52	23	1-pentene	21796	9550	21796	-	2.1	10.7
13.56	37	2-methylpentane	32593	12345	32593	-	2.2	11.2
13.68	40	butanal	33282	13242	33282	-	5.9	23.8
13.81	40b	2-butanone	20632	6111	20632	-	3.4	13.6
14.07	43	2-methyl-1-pentene	35337	12031	35337	-	19.9	119.5
14.2	?	?	21071	8352	-	21071	-	-
14.52	44	n-hexane	32223	14041	32223	-	2.3	13.5
14.64	?	?	22558	9936	-	22558	-	-
14.89	?	?	22529	9747	-	22529	-	-
15.26	49	2,4-dimethylpentane	28018	11638	28018	-	1.7	12.0
15.31	?	?	32066	13995	-	32066	-	-
15.89	52	benzene	31562	11447	31562	-	2.3	14.0
16.12	54	cyclohexane	29506	11365	29506	-	2.1	12.8
16.24	55	2-methylhexane	38716	16521	38716	-	2.4	16.9
16.32	56	2,3-dimethylpentane	32261	13612	32261	-	2.0	14.2
16.46	57	3-methylhexane	39517	15339	39517	-	2.0	13.8
16.81	58	2,2,4-trimethylpentane	36992	15320	36992	-	2.3	18.8
16.97	59	ISTD 2	281436	107446	-	-	-	-
17.65	63	methylcyclohexane/ MIBK	31664	11875	31664	-	2.0	14.2
18.32	65	2,3,4-trimethylpentane	34663	12893	34663	-	2.3	18.1
18.49	66	toluene	30478	10825	30478	-	2.0	14.1
18.63	67	2-methylheptane	33460	12977	33460	-	2.1	16.8
18.83	68	3-methylheptane	36296	12895	36296	-	2.4	18.8

19.48	70	n-octane	32873	12551	32873	-	1.9	15.1
21.01	71	ethylbenzene	25421	8248	25421	-	1.5	11.7
21.24	72	p-xylene & m-xylene	44079	10630	44079	-	3.0	24.3
21.92	76	o-xylene	21685	6623	21685	-	1.6	12.4
22.19	77	n-nonane	37504	10448	37504	-	2.1	19.2
22.49	?	?	6021	1008	-	6021	-	-
22.62	78	ISTD 3	28251	7650	-	-	-	-
22.84	79	isopropylbenzene	20147	5981	20147	-	1.7	15.1
23.73	83	n-propylbenzene	21479	5660	21479	-	1.8	16.4
29.9	?	?	18561	1613	-	18561	-	-
					1087440	371822	154.8	733.0

Total Area	1E+06
Area of Knowns	1E+06
Area of Unknowns	371822
Total Area/Known Area	1.342
Known ppbC	733
Total ppbC	984

Peak Report -- Channel A
36173
0.68155
Smog Chamber
c:\sarah\1-1
c:\ezchrom\methods\0to15.met
System
Peaks 55

RT (min)	Peak ID	Compound	Paraffin (ppbC)	Olefin (ppbC)	Aromatic (ppbC)	Carbonyl (ppbC)	Alcohol (ppbC)
6.557	5	propane	8.1	0.0	0.0	0.0	0.0
6.637	?	?	-	-	-	-	-
7.877	9	ISTD 1	-	-	-	-	-
8.317	11b	1,3-butadiene	-	-	-	-	-
8.477	?	?	-	-	-	-	-
8.71	?	?	-	-	-	-	-
9.01	?	?	-	-	-	-	-
9.413	?	?	-	-	-	-	-
10.353	19	ethanol	0.0	0.0	0.0	0.0	22.9
10.5	?	?	-	-	-	-	-
10.697	20b	2-propenal	0.0	0.0	0.0	11.8	0.0
10.88	21	isopentane	22.6	0.0	0.0	0.0	0.0
10.96	22b	acetone/propanal	0.0	0.0	0.0	141.1	0.0
11.333	?	?	-	-	-	-	-
11.667	?	?	-	-	-	-	-
11.81	24	n-pentane	6.8	0.0	0.0	0.0	0.0
11.907	25	isoprene	0.0	11.2	0.0	0.0	0.0
12.133	26b	1,1-dichloroethylene	-	-	-	-	-
12.273	27	cis-2-pentene	0.0	5.2	0.0	0.0	0.0
12.707	?	?	-	-	-	-	-
13.213	?	?	-	-	-	-	-
13.313	?	?	-	-	-	-	-
13.52	23	1-pentene	0.0	10.7	0.0	0.0	0.0
13.56	37	2-methylpentane	11.2	0.0	0.0	0.0	0.0
13.677	40	butanal	0.0	0.0	0.0	23.8	0.0
13.807	40b	2-butanone	0.0	0.0	0.0	13.6	0.0
14.07	43	2-methyl-1-pentene	0.0	119.5	0.0	0.0	0.0
14.2	?	?	-	-	-	-	-
14.52	44	n-hexane	13.5	0.0	0.0	0.0	0.0
14.643	?	?	-	-	-	-	-
14.893	?	?	-	-	-	-	-
15.257	49	2,4-dimethylpentane	12.0	0.0	0.0	0.0	0.0
15.313	?	?	-	-	-	-	-
15.893	52	benzene	0.0	0.0	14.0	0.0	0.0
16.123	54	cyclohexane	12.8	0.0	0.0	0.0	0.0
16.24	55	2-methylhexane	16.9	0.0	0.0	0.0	0.0
16.317	56	2,3-dimethylpentane	14.2	0.0	0.0	0.0	0.0
16.46	57	3-methylhexane	13.8	0.0	0.0	0.0	0.0
16.81	58	2,2,4-trimethylpentane	18.8	0.0	0.0	0.0	0.0
16.967	59	ISTD 2	-	-	-	-	-
17.65	63	methylcyclohexane/MIBK	14.2	0.0	0.0	0.0	0.0
18.32	65	2,3,4-trimethylpentane	18.1	0.0	0.0	0.0	0.0
18.49	66	toluene	0.0	0.0	14.1	0.0	0.0
18.627	67	2-methylheptane	16.8	0.0	0.0	0.0	0.0

18.833	68	3-methylheptane	18.8	0.0	0.0	0.0	0.0
19.48	70	n-octane	15.1	0.0	0.0	0.0	0.0
21.01	71	ethylbenzene	0.0	0.0	11.7	0.0	0.0
21.243	72	p-xylene & m-xylene	0.0	0.0	24.3	0.0	0.0
21.92	76	o-xylene	0.0	0.0	12.4	0.0	0.0
22.187	77	n-nonane	19.2	0.0	0.0	0.0	0.0
22.49	?	?	-	-	-	-	-
22.62	78	ISTD 3	-	-	-	-	-
22.837	79	isopropylbenzene	0.0	0.0	15.1	0.0	0.0
23.733	83	n-propylbenzene	0.0	0.0	16.4	0.0	0.0
29.9	?	?	-	-	-	-	-
			253.1	146.6	107.9	190.2	22.9

Peak Report -- Channel A

		RT (min)
0.65	ISTD 1	7.867
Smog Chamber	ISTD 2	16.967
c:\sarah\1-2	ISTD 3	22.62

c:\ezchrom\methods\0to15.met
System
Peaks 47

RT (min)	Peak ID	Compound	Area	Height	Area of Knowns	Area of Unknowns	Conc (ppbv)	ppbC
6.55	5	propane	9388	3076	9388	-	1.4	4.1
6.63	?	?	12718	4110	-	12718	-	-
7.87	9	ISTD 1	212479	62937	-	-	-	-
8.3	11b	1,3-butadiene	19155	4585	19155	-	1.1	4.6
8.47	?	?	12278	3052	-	12278	-	-
8.7	?	?	18923	6518	-	18923	-	-
10.4	19	ethanol	7671	2918	7671	-	3.3	6.6
10.5	?	?	10688	1872	-	10688	-	-
10.7	20b	2-propenal	13637	4693	13637	-	4.2	12.7
10.9	21	isopentane	35963	14767	35963	-	3.4	17.0
10.9	21	isopentane	156826	36182	156826	-	14.8	74.2
11.3	?	?	7818	2748	-	7818	-	-
11.7	?	?	18203	7357	-	18203	-	-
12.7	?	?	25280	9542	-	25280	-	-
13.3	?	?	18256	4017	-	18256	-	-
13.5	23	1-pentene	15717	7110	15717	-	1.6	7.8
13.6	37	2-methylpentane	25218	9242	25218	-	1.7	8.7
13.7	40	butanal	26785	10582	26785	-	4.8	19.1
13.8	40b	2-butanone	12259	2597	12259	-	2.0	8.1
14.1	43	2-methyl-1-pentene	40490	11218	40490	-	22.8	137.0
14.5	44	n-hexane	20641	9043	20641	-	1.4	8.7
15.3	49	2,4-dimethylpentane	18603	7922	18603	-	1.1	8.0
15.3	?	?	24622	10437	-	24622	-	-
15.9	52	benzene	31504	11340	31504	-	2.3	13.9
16.1	54	cyclohexane	20432	7798	20432	-	1.5	8.9
16.2	55	2-methylhexane	29831	12494	29831	-	1.9	13.0
16.3	56	2,3-dimethylpentane	22547	9413	22547	-	1.4	10.0
16.5	57	3-methylhexane	32534	11236	32534	-	1.6	11.4
16.8	58	2,2,4-trimethylpentane	29603	12142	29603	-	1.9	15.0
17	59	ISTD 2	270676	105706	-	-	-	-
17.7	63	methylcyclohexane/MIBK	21643	7402	21643	-	1.4	9.7
18.3	65	2,3,4-trimethylpentane	26427	8771	26427	-	1.7	13.8
18.5	66	toluene	26682	9078	26682	-	1.8	12.4
18.6	67	2-methylheptane	22041	8195	22041	-	1.4	11.1
18.8	68	3-methylheptane	27296	8413	27296	-	1.8	14.1
19.5	70	n-octane	21858	7787	21858	-	1.3	10.1
21	71	ethylbenzene	18052	5756	18052	-	1.0	8.3
21.3	72	p-xylene & m-xylene	18917	4624	18917	-	1.3	10.4
21.9	76	o-xylene	11618	3467	11618	-	0.8	6.7
22.2	77	n-nonane	17527	4718	17527	-	1.0	9.0
22.5	?	?	8958	1270	-	8958	-	-
22.6	78	ISTD 3	29174	7696	-	-	-	-
22.8	79	isopropylbenzene	11908	3390	11908	-	1.0	8.9

23.7	83	n-propylbenzene	13640	3060	13640	-	1.2	10.4
28.8	?	?	6716	557	-	6716	-	-
29.9	?	?	22883	1763	-	22883	-	-
32.9	?	?	5043	604	-	5043	-	-
					806413	192386	90.0	513.4

Total Area	998799
Area of Knowns	806413
Area of Unknowns	192386
Total Area/Known Area	1.239
Known ppbC	513
Total ppbC	636

Peak Report -- Channel A
36173
0.65
Smog Chamber
c:\sarah\1-2
c:\ezchrom\methods\0to15.met
System
Peaks

RT (min)	Peak ID	Compound	Paraffin (ppbC)	Olefin (ppbC)	Aromatic (ppbC)	Carbonyl (ppbC)	Alcohol (ppbC)
6.55	5	propane	4.1	0.0	0.0	0.0	0.0
6.63	?	?	-	-	-	-	-
7.867	9	ISTD 1	-	-	-	-	-
8.297	11b	1,3-butadiene	-	-	-	-	-
8.467	?	?	-	-	-	-	-
8.703	?	?	-	-	-	-	-
10.35	19	ethanol	0.0	0.0	0.0	0.0	6.6
10.48	?	?	-	-	-	-	-
10.69	20b	2-propenal	0.0	0.0	0.0	12.7	0.0
10.88	21	isopentane	17.0	0.0	0.0	0.0	0.0
10.94	21	isopentane	74.2	0.0	0.0	0.0	0.0
11.33	?	?	-	-	-	-	-
11.66	?	?	-	-	-	-	-
12.7	?	?	-	-	-	-	-
13.31	?	?	-	-	-	-	-
13.52	23	1-pentene	0.0	7.8	0.0	0.0	0.0
13.56	37	2-methylpentane	8.7	0.0	0.0	0.0	0.0
13.68	40	butanal	0.0	0.0	0.0	19.1	0.0
13.81	40b	2-butanone	0.0	0.0	0.0	8.1	0.0
14.07	43	2-methyl-1-pentene	0.0	137.0	0.0	0.0	0.0
14.52	44	n-hexane	8.7	0.0	0.0	0.0	0.0
15.26	49	2,4-dimethylpentane	8.0	0.0	0.0	0.0	0.0
15.31	?	?	-	-	-	-	-
15.89	52	benzene	0.0	0.0	13.9	0.0	0.0
16.12	54	cyclohexane	8.9	0.0	0.0	0.0	0.0
16.24	55	2-methylhexane	13.0	0.0	0.0	0.0	0.0
16.32	56	2,3-dimethylpentane	10.0	0.0	0.0	0.0	0.0
16.46	57	3-methylhexane	11.4	0.0	0.0	0.0	0.0
16.81	58	2,2,4-trimethylpentane	15.0	0.0	0.0	0.0	0.0
16.97	59	ISTD 2	-	-	-	-	-
17.65	63	methylcyclohexane/MIBK	9.7	0.0	0.0	0.0	0.0
18.32	65	2,3,4-trimethylpentane	13.8	0.0	0.0	0.0	0.0
18.49	66	toluene	0.0	0.0	12.4	0.0	0.0
18.63	67	2-methylheptane	11.1	0.0	0.0	0.0	0.0
18.83	68	3-methylheptane	14.1	0.0	0.0	0.0	0.0
19.48	70	n-octane	10.1	0.0	0.0	0.0	0.0
21.01	71	ethylbenzene	0.0	0.0	8.3	0.0	0.0
21.25	72	p-xylene & m-xylene	0.0	0.0	10.4	0.0	0.0
21.92	76	o-xylene	0.0	0.0	6.7	0.0	0.0
22.19	77	n-nonane	9.0	0.0	0.0	0.0	0.0
22.47	?	?	-	-	-	-	-
22.62	78	ISTD 3	-	-	-	-	-
22.84	79	isopropylbenzene	0.0	0.0	8.9	0.0	0.0
23.73	83	n-propylbenzene	0.0	0.0	10.4	0.0	0.0
28.77	?	?	-	-	-	-	-

29.87	?	?	-	-	-	-	-
32.94	?	?	-	-	-	-	-
			246.6	144.7	71.0	39.9	6.6

Peak Report -- Channel A

		RT (min)
0.62	ISTD 1	7.853
Smog Chamber	ISTD 2	16.95
c:\sarah\2-1	ISTD 3	22.61

c:\ezchrom\methods\0to15.met
System
Peaks 59

RT (min)	Peak ID	Compound	Area	Height	Area of Knowns	Area of Unknowns	Conc (ppbv)	ppbC
6.54	5	propane	24974	8204	24974	-	3.7	11.0
6.62	?	?	19279	6276	-	19279	-	-
7.85	9	ISTD 1	205362	58275	-	-	-	-
8.29	11b	1,3-butadiene	15017	3763	15017	-	0.9	3.6
8.46	?	?	34470	11077	-	34470	-	-
8.69	?	?	32059	11305	-	32059	-	-
8.99	?	?	31620	11436	-	31620	-	-
9.39	?	?	26436	9799	-	26436	-	-
10.3	19	ethanol	38326	14594	38326	-	16.4	32.8
10.5	?	?	9754	1733	-	9754	-	-
10.7	20b	2-propenal	15048	5201	15048	-	4.7	14.1
10.9	21	isopentane	69973	26941	69973	-	6.6	33.1
10.9	22b	acetone/propanal	112152	31038	112152	-	46.9	140.6
11.3	?	?	36202	14453	-	36202	-	-
11.6	?	?	34320	14097	-	34320	-	-
11.8	25	isoprene	22667	9027	22667	-	2.3	11.3
11.9	?	?	33015	13786	-	33015	-	-
12.1	26b	1,1-dichloroethylene	32347	13055	32347	-	6.6	13.3
12.3	27	cis-2-pentene	20624	8401	20624	-	1.6	7.8
12.7	?	?	42932	16525	-	42932	-	-
13.2	?	?	36151	12802	-	36151	-	-
13.3	?	?	44657	17196	-	44657	-	-
13.5	23	1-pentene	31225	14168	31225	-	3.1	15.4
13.5	37	2-methylpentane	47878	18153	47878	-	3.3	16.4
13.7	40	butanal	51633	20835	51633	-	9.2	36.9
13.8	40b	2-butanone	27296	7910	27296	-	4.5	18.0
14.1	43	2-methyl-1-pentene	47669	17809	47669	-	26.9	161.3
14.2	?	?	30805	12379	-	30805	-	-
14.5	44	n-hexane	42762	18674	42762	-	3.0	18.0
14.6	?	?	33732	14972	-	33732	-	-
14.9	?	?	33939	14710	-	33939	-	-
15.2	49	2,4-dimethylpentane	39992	17285	39992	-	2.4	17.1
15.3	?	?	49228	20843	-	49228	-	-
15.9	52	benzene	50191	19041	50191	-	3.7	22.2
16.1	54	cyclohexane	43443	16814	43443	-	3.2	18.9
16.2	55	2-methylhexane	57037	24620	57037	-	3.6	24.9
16.3	56	2,3-dimethylpentane	48144	20357	48144	-	3.0	21.3
16.4	57	3-methylhexane	57620	21791	57620	-	2.9	20.2
16.8	58	2,2,4-trimethylpentane	54981	22700	54981	-	3.5	27.9
17	59	ISTD 2	280558	1E+05	-	-	-	-
17	60	n-heptane	18633	20265	18633	-	1.2	8.1
17.6	63	methylcyclohexane/ MIBK	47236	17867	47236	-	3.0	21.2
18.1	?	?	5740	1040	-	5740	-	-
18.3	65	2,3,4-	51626	19431	51626	-	3.4	27.0

		trimethylpentane						
18.5	66	toluene	49478	17424	49478	-	3.3	22.9
18.6	67	2-methylheptane	50935	19757	50935	-	3.2	25.6
18.8	68	3-methylheptane	55215	19539	55215	-	3.6	28.6
19.5	70	n-octane	50539	19212	50539	-	2.9	23.2
21	71	ethylbenzene	42960	14133	42960	-	2.5	19.7
21.2	72	p-xylene & m-xylene	78095	18558	78095	-	5.4	43.1
21.9	76	o-xylene	37996	11774	37996	-	2.7	21.8
22.2	77	n-nonane	53418	16921	53418	-	3.0	27.3
22.6	78	ISTD 3	28406	7923	-	-	-	-
22.8	79	isopropylbenzene	35417	10727	35417	-	2.9	26.5
23.7	83	n-propylbenzene	37053	10449	37053	-	3.1	28.3
24.1	85	1,3,5-trimethylbenzene	7620	2238	7620	-	0.8	7.1
25	89	1,2,4-trimethylbenzene	14212	3753	14212	-	1.6	14.5
29.8	?	?	26597	2219	-	26597	-	-
30.1	?	?	19368	1425	-	19368	-	-
					1581432	580304	204.4	1030.7

Total Area	2E+06
Area of Knowns	2E+06
Area of Unknowns	580304
Total Area/Known Area	1.367
Known ppbC	1031
Total ppbC	1409

0.6182
Smog Chamber
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System
Peaks

RT (min)	Peak ID	Compound	Paraffin (ppbC)	Olefin (ppbC)	Aromatic (ppbC)	Carbonyl (ppbC)	Alcohol (ppbC)
6.54	5	propane	11.0	0.0	0.0	0.0	0.0
6.62	?	?	-	-	-	-	-
7.853	9	ISTD 1	-	-	-	-	-
8.29	11b	1,3-butadiene	-	-	-	-	-
8.457	?	?	-	-	-	-	-
8.687	?	?	-	-	-	-	-
8.99	?	?	-	-	-	-	-
9.393	?	?	-	-	-	-	-
10.337	19	ethanol	0.0	0.0	0.0	0.0	32.8
10.47	?	?	-	-	-	-	-
10.673	20b	2-propenal	0.0	0.0	0.0	14.1	0.0
10.863	21	isopentane	33.1	0.0	0.0	0.0	0.0
10.937	22b	acetone/propanal	0.0	0.0	0.0	140.6	0.0
11.317	?	?	-	-	-	-	-
11.647	?	?	-	-	-	-	-
11.793	25	isoprene	0.0	11.3	0.0	0.0	0.0
11.89	?	?	-	-	-	-	-
12.117	26b	1,1-dichloroethylene	-	-	-	-	-
12.257	27	cis-2-pentene	0.0	7.8	0.0	0.0	0.0
12.69	?	?	-	-	-	-	-
13.197	?	?	-	-	-	-	-
13.297	?	?	-	-	-	-	-
13.503	23	1-pentene	0.0	15.4	0.0	0.0	0.0
13.547	37	2-methylpentane	16.4	0.0	0.0	0.0	0.0
13.663	40	butanal	0.0	0.0	0.0	36.9	0.0
13.787	40b	2-butanone	0.0	0.0	0.0	18.0	0.0
14.053	43	2-methyl-1-pentene	0.0	161.3	0.0	0.0	0.0
14.187	?	?	-	-	-	-	-
14.507	44	n-hexane	18.0	0.0	0.0	0.0	0.0
14.63	?	?	-	-	-	-	-
14.88	?	?	-	-	-	-	-
15.247	49	2,4-dimethylpentane	17.1	0.0	0.0	0.0	0.0
15.3	?	?	-	-	-	-	-
15.88	52	benzene	0.0	0.0	22.2	0.0	0.0
16.11	54	cyclohexane	18.9	0.0	0.0	0.0	0.0
16.23	55	2-methylhexane	24.9	0.0	0.0	0.0	0.0
16.303	56	2,3-dimethylpentane	21.3	0.0	0.0	0.0	0.0
16.447	57	3-methylhexane	20.2	0.0	0.0	0.0	0.0
16.797	58	2,2,4-trimethylpentane	27.9	0.0	0.0	0.0	0.0
16.953	59	ISTD 2	-	-	-	-	-
17.007	60	n-heptane	8.1	0.0	0.0	0.0	0.0
17.637	63	methylcyclohexane/MIBK	21.2	0.0	0.0	0.0	0.0
18.09	?	?	-	-	-	-	-
18.307	65	2,3,4-trimethylpentane	27.0	0.0	0.0	0.0	0.0
18.48	66	toluene	0.0	0.0	22.9	0.0	0.0
18.613	67	2-methylheptane	25.6	0.0	0.0	0.0	0.0
18.82	68	3-methylheptane	28.6	0.0	0.0	0.0	0.0

19.467	70	n-octane	23.2	0.0	0.0	0.0	0.0
20.993	71	ethylbenzene	0.0	0.0	19.7	0.0	0.0
21.227	72	p-xylene & m-xylene	0.0	0.0	43.1	0.0	0.0
21.903	76	o-xylene	0.0	0.0	21.8	0.0	0.0
22.173	77	n-nonane	27.3	0.0	0.0	0.0	0.0
22.607	78	ISTD 3	-	-	-	-	-
22.82	79	isopropylbenzene	0.0	0.0	26.5	0.0	0.0
23.717	83	n-propylbenzene	0.0	0.0	28.3	0.0	0.0
24.14	85	1,3,5-trimethylbenzene	0.0	0.0	7.1	0.0	0.0
24.98	89	1,2,4-trimethylbenzene	0.0	0.0	14.5	0.0	0.0
29.817	?	?	-	-	-	-	-
30.12	?	?	-	-	-	-	-
			369.8	195.7	206.1	209.5	32.8

Peak Report -- Channel A

36173		RT (min)
0.5546	ISTD 1	7.757
Smog Chamber	ISTD 2	16.89
c:\sarah\2-2	ISTD 3	22.54
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System		
Peaks 54		

RT (min)	Peak ID	Compound	Area	Height	Area of Knowns	Area of Unknowns	Conc (ppbv)	ppbC
6.45	5	propane	6095	2091	6095	-	0.9	2.7
6.53	?	?	12613	4244	-	12613	-	-
7.757	9	ISTD 1	278771	86708	-	-	-	-
8.18	11b	1,3-butadiene	24753	5734	24753	-	1.5	5.9
8.35	12	n-butane	9116	2317	9116	-	1.1	4.2
8.603	?	?	18392	6566	-	18392	-	-
8.907	?	?	5389	1743	-	5389	-	-
10.337	?	?	18667	2653	-	18667	-	-
10.583	20b	2-propenal	19742	7011	19742	-	6.1	18.4
10.817	21	isopentane	268688	53464	268688	-	25.4	127.0
11.577	?	?	15639	6507	-	15639	-	-
11.89	26	trans-2-pentene	5088	768	5088	-	0.5	2.5
12.617	?	?	25465	9450	-	25465	-	-
12.83	?	?	11280	3899	-	11280	-	-
13.073	?	?	8667	1680	-	8667	-	-
13.157	?	?	12697	2560	-	12697	-	-
13.43	36	2-methoxy-2-methyl propane	18636	7184	18636	-	2.3	11.5
13.473	23	1-pentene	20988	8042	20988	-	2.1	10.3
13.59	40	butanal	40718	15140	40718	-	7.3	29.1
13.703	?	?	38718	14362	-	38718	-	-
13.913	41	3-methylpentane	18087	6172	18087	-	1.5	8.8
13.977	?	?	32100	9982	-	32100	-	-
14.317	?	?	5913	2231	-	5913	-	-
14.437	44	n-hexane	16880	7488	16880	-	1.2	7.1
15.177	49	2,4-dimethylpentane	13867	5893	13867	-	0.8	5.9
15.233	49	2,4-dimethylpentane	25038	9395	25038	-	1.5	10.7
15.67	?	?	8701	2100	-	8701	-	-
15.81	52	benzene	44963	17403	44963	-	3.3	19.9
16.043	54	cyclohexane	17228	6467	17228	-	1.2	7.5
16.16	55	2-methylhexane	39032	15602	39032	-	2.4	17.0
16.24	56	2,3-dimethylpentane	17331	7083	17331	-	1.1	7.7
16.32	?	?	14601	5048	-	14601	-	-
16.383	57	3-methylhexane	27478	7072	27478	-	1.4	9.6
16.733	58	2,2,4-trimethylpentane	26918	10733	26918	-	1.7	13.7
16.893	59	ISTD 2	271160	1E+05	-	-	-	-
17.25	?	?	6547	1262	-	6547	-	-
17.573	63	methylcyclohexane/MIBK	13820	4788	13820	-	0.9	6.2
18.243	65	2,3,4-trimethylpentane	18983	6731	18983	-	1.2	9.9
18.413	66	toluene	39684	13568	39684	-	2.6	18.4
18.553	67	2-methylheptane	13745	5379	13745	-	0.9	6.9
18.76	68	3-methylheptane	23947	5849	23947	-	1.6	12.4
19.403	70	n-octane	12310	4576	12310	-	0.7	5.7
20.93	71	ethylbenzene	24719	8135	24719	-	1.4	11.3

21.173	72	p-xylene & m-xylene	21963	5465	21963	-	1.5	12.1
21.843	76	o-xylene	14063	4270	14063	-	1.0	8.1
22.11	77	n-nonane	29869	7828	29869	-	1.7	15.3
22.543	78	ISTD 3	38477	11607	-	-	-	-
22.76	79	isopropylbenzene	21255	6444	21255	-	1.8	15.9
23.653	83	n-propylbenzene	20861	4991	20861	-	1.8	15.9
25.657	?	?	9269	918	-	9269	-	-
27.003	?	?	10765	1568	-	10765	-	-
30.03	?	?	7407	334	-	7407	-	-
34.15	?	?	13282	1546	-	13282	-	-
34.64	?	?	5991	729	-	5991	-	-
					915865	282103	80.4	457.7

Total Area	1E+06
Area of Knowns	915865
Area of Unknowns	282103

Peak Report -- Channel A
36173
0.555
Smog Chamber
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System
Peaks

RT (min)	Peak ID	Compound	Paraffin (ppbC)	Olefin (ppbC)	Aromatic (ppbC)	Carbonyl (ppbC)	Alcohol (ppbC)
6.45	5	propane	2.7	0.0	0.0	0.0	0.0
6.53	?	?	-	-	-	-	-
7.757	9	ISTD 1	-	-	-	-	-
8.18	11b	1,3-butadiene	-	-	-	-	-
8.35	12	n-butane	4.2	0.0	0.0	0.0	0.0
8.603	?	?	-	-	-	-	-
8.907	?	?	-	-	-	-	-
10.34	?	?	-	-	-	-	-
10.58	20b	2-propenal	0.0	0.0	0.0	18.4	0.0
10.82	21	isopentane	127.0	0.0	0.0	0.0	0.0
11.58	?	?	-	-	-	-	-
11.89	26	trans-2-pentene	0.0	2.5	0.0	0.0	0.0
12.62	?	?	-	-	-	-	-
12.83	?	?	-	-	-	-	-
13.07	?	?	-	-	-	-	-
13.16	?	?	-	-	-	-	-
13.43	36	2-methoxy-2-methyl propane	-	-	-	-	-
13.47	23	1-pentene	0.0	10.3	0.0	0.0	0.0
13.59	40	butanal	0.0	0.0	0.0	29.1	0.0
13.7	?	?	-	-	-	-	-
13.91	41	3-methylpentane	8.8	0.0	0.0	0.0	0.0
13.98	?	?	-	-	-	-	-
14.32	?	?	-	-	-	-	-
14.44	44	n-hexane	7.1	0.0	0.0	0.0	0.0
15.18	49	2,4-dimethylpentane	5.9	0.0	0.0	0.0	0.0
15.23	49	2,4-dimethylpentane	10.7	0.0	0.0	0.0	0.0
15.67	?	?	-	-	-	-	-
15.81	52	benzene	0.0	0.0	19.9	0.0	0.0
16.04	54	cyclohexane	7.5	0.0	0.0	0.0	0.0
16.16	55	2-methylhexane	17.0	0.0	0.0	0.0	0.0
16.24	56	2,3-dimethylpentane	7.7	0.0	0.0	0.0	0.0
16.32	?	?	-	-	-	-	-
16.38	57	3-methylhexane	9.6	0.0	0.0	0.0	0.0
16.73	58	2,2,4-trimethylpentane	13.7	0.0	0.0	0.0	0.0
16.89	59	ISTD 2	-	-	-	-	-
17.25	?	?	-	-	-	-	-
17.57	63	methylcyclohexane/MIBK	6.2	0.0	0.0	0.0	0.0
18.24	65	2,3,4-trimethylpentane	9.9	0.0	0.0	0.0	0.0
18.41	66	toluene	0.0	0.0	18.4	0.0	0.0
18.55	67	2-methylheptane	6.9	0.0	0.0	0.0	0.0
18.76	68	3-methylheptane	12.4	0.0	0.0	0.0	0.0
19.4	70	n-octane	5.7	0.0	0.0	0.0	0.0
20.93	71	ethylbenzene	0.0	0.0	11.3	0.0	0.0
21.17	72	p-xylene & m-xylene	0.0	0.0	12.1	0.0	0.0

21.84	76	o-xylene	0.0	0.0	8.1	0.0	0.0
22.11	77	n-nonane	15.3	0.0	0.0	0.0	0.0
22.54	78	ISTD 3	-	-	-	-	-
22.76	79	isopropylbenzene	0.0	0.0	15.9	0.0	0.0
23.65	83	n-propylbenzene	0.0	0.0	15.9	0.0	0.0
25.66	?	?	-	-	-	-	-
27	?	?	-	-	-	-	-
30.03	?	?	-	-	-	-	-
34.15	?	?	-	-	-	-	-
34.64	?	?	-	-	-	-	-
			278.3	12.9	101.6	47.5	0.0

Peak Report -- Channel A

36174		RT (min)
0.664	ISTD 1	7.85
smog chamber	ISTD 2	16.95
c:\sarah\3-1	ISTD 3	22.603
c:\ezchrom\methods\0to15.met		
System		
Peaks 72		

RT (min)	Peak ID	Compound	Area	Height	Area of Knowns	Area of Unknowns	Conc (ppbv)	ppbC
6.547	5	propane	20837	6763	20837	-	3.1	9.2
6.627	?	?	12398	4113	-	12398	-	-
7.85	9	ISTD 1	242245	73267	-	-	-	-
8.283	11b	1,3-butadiene	12550	2491	12550	-	0.7	3.0
8.45	?	?	46198	12269	-	46198	-	-
8.7	?	?	20488	7149	-	20488	-	-
9.003	14	bromomethane	20604	7300	20604	-	9.6	9.6
9.407	?	?	16529	6182	-	16529	-	-
10.35	19	ethanol	35434	9761	35434	-	15.2	30.3
10.66	20b	2-propenal	22382	7868	22382	-	7.0	20.9
10.92	21	isopentane	509584	117074	509584	-	48.2	240.9
11.32	?	?	24825	9214	-	24825	-	-
11.65	?	?	21544	8803	-	21544	-	-
11.8	25	isoprene	21343	8037	21343	-	2.1	10.6
11.9	?	?	22529	8956	-	22529	-	-
12.12	26b	1,1-dichloroethylene	19961	8120	19961	-	4.1	8.2
12.26	27	cis-2-pentene	22022	9026	22022	-	1.7	8.3
12.69	?	?	30075	10437	-	30075	-	-
12.9	31	cyclopentene	72807	13301	72807	-	5.3	26.7
13.2	?	?	28191	9044	-	28191	-	-
13.3	?	?	25240	10270	-	25240	-	-
13.41	35	2,3-dimethylbutane	19811	4934	19811	-	1.4	8.5
13.51	23	1-pentene	21942	8862	21942	-	2.2	10.8
13.55	37	2-methylpentane	26581	10735	26581	-	1.8	9.1
13.66	40	butanal	46722	17727	46722	-	8.3	33.4
13.77	?	?	585599	227613	-	585599	-	-
13.96	41	3-methylpentane	17704	6857	17704	-	1.4	8.6
14.03	?	?	130224	44708	-	130224	-	-
14.18	?	?	21823	8873	-	21823	-	-
14.38	?	?	6944	2390	-	6944	-	-
14.5	44	n-hexane	27407	11823	27407	-	1.9	11.5
14.63	?	?	24589	10326	-	24589	-	-
14.88	?	?	24184	10337	-	24184	-	-
15.24	49	2,4-dimethylpentane	71590	26118	71590	-	4.4	30.6
15.29	?	?	34943	15165	-	34943	-	-
15.48	?	?	6531	2137	-	6531	-	-
15.69	?	?	17083	4574	-	17083	-	-
15.88	52	benzene	30748	11412	30748	-	2.3	13.6
16.1	54	cyclohexane	29309	10772	29309	-	2.1	12.8
16.22	55	2-methylhexane	35960	15675	35960	-	2.2	15.7
16.3	56	2,3-dimethylpentane	46138	13966	46138	-	2.9	20.4
16.45	57	3-methylhexane	58881	20637	58881	-	2.9	20.6
16.79	58	2,2,4-trimethylpentane	39139	14285	39139	-	2.5	19.9
16.95	59	ISTD 2	327732	127887	-	-	-	-
17.31	?	?	38035	15434	-	38035	-	-
17.63	63	methylcyclohexane/MI	39488	11159	39488	-	2.5	17.7

		BK						
17.83	?	?	5614	1493	-	5614	-	-
18.2	64	1,1,2-trichloroethane	6267	2214	6267	-	1.4	2.9
18.3	65	2,3,4-trimethylpentane	30164	11327	30164	-	2.0	15.8
18.48	66	toluene	29393	9763	29393	-	1.9	13.6
18.61	67	2-methylheptane	33795	12206	33795	-	2.1	17.0
18.72	?	?	46762	14618	-	46762	-	-
18.82	68	3-methylheptane	32640	11808	32640	-	2.1	16.9
18.97	69	hexanal	25810	8723	25810	-	4.0	23.9
19.46	70	n-octane	35015	12247	35015	-	2.0	16.1
20.36	?	?	5485	918	-	5485	-	-
20.99	71	ethylbenzene	33496	9227	33496	-	1.9	15.4
21.23	72	p-xylene & m-xylene	51900	10933	51900	-	3.6	28.6
21.43	?	?	7538	2272	-	7538	-	-
21.7	75	styrene	41571	8463	41571	-	11.8	94.1
21.9	76	o-xylene	23653	6667	23653	-	1.7	13.5
22.17	77	n-nonane	42142	12599	42142	-	2.4	21.6
22.6	78	ISTD 3	83361	24332	-	-	-	-
22.82	79	isopropylbenzene	22257	6711	22257	-	1.8	16.6
23.32	?	?	6057	1380	-	6057	-	-
23.49	81	benzaldehyde/alpha-pinene	41997	9581	41997	-	1.9	19.3
23.72	83	n-propylbenzene	28902	6879	28902	-	2.4	22.0
24.14	85	1,3,5-trimethylbenzene	17543	5101	17543	-	1.8	16.5
24.83	88	beta-pinene	24865	6350	24865	-	1.8	0.0
24.98	89	1,2,4-trimethylbenzene	17537	4925	17537	-	2.0	17.9
26.79	95	m-diethylbenzene	8650	2328	8650	-	1.6	16.1
30.29	?	?	7716	951	-	7716	-	-
					1816541	1217144	186.3	988.6

Total Area	3E+06
Area of Knowns	2E+06
Area of Unknowns	1E+06
Total Area/Known Area	1.670
Known ppbC	989
Total ppbC	1651

Peak Report -- Channel A
36174
0.664
smog chamber
c:\sarah\3-1
c:\ezchrom\methods\0to15.met
Syste
m
Peaks

RT (min)	Peak ID	Compound	Paraffin (ppbC)	Olefin (ppbC)	Aromatic (ppbC)	Carbonyl (ppbC)	Alcohol (ppbC)
6.547	5	propane	9.2	0.0	0.0	0.0	0.0
6.627	?	?	-	-	-	-	-
7.85	9	ISTD 1	-	-	-	-	-
8.283	11b	1,3-butadiene	-	-	-	-	-
8.45	?	?	-	-	-	-	-
8.7	?	?	-	-	-	-	-
9.003	14	bromomethane	-	-	-	-	-
9.407	?	?	-	-	-	-	-
10.35	19	ethanol	0.0	0.0	0.0	0.0	30.3
10.66	20b	2-propenal	0.0	0.0	0.0	20.9	0.0
10.92	21	isopentane	240.9	0.0	0.0	0.0	0.0
11.32	?	?	-	-	-	-	-
11.65	?	?	-	-	-	-	-
11.8	25	isoprene	0.0	10.6	0.0	0.0	0.0
11.9	?	?	-	-	-	-	-
12.12	26b	1,1-dichloroethylene	-	-	-	-	-
12.26	27	cis-2-pentene	0.0	8.3	0.0	0.0	0.0
12.69	?	?	-	-	-	-	-
12.9	31	cyclopentene	-	-	-	-	-
13.2	?	?	-	-	-	-	-
13.3	?	?	-	-	-	-	-
13.41	35	2,3-dimethylbutane	8.5	0.0	0.0	0.0	0.0
13.51	23	1-pentene	0.0	10.8	0.0	0.0	0.0
13.55	37	2-methylpentane	9.1	0.0	0.0	0.0	0.0
13.66	40	butanal	0.0	0.0	0.0	33.4	0.0
13.77	?	?	-	-	-	-	-
13.96	41	3-methylpentane	8.6	0.0	0.0	0.0	0.0
14.03	?	?	-	-	-	-	-
14.18	?	?	-	-	-	-	-
14.38	?	?	-	-	-	-	-
14.5	44	n-hexane	11.5	0.0	0.0	0.0	0.0
14.63	?	?	-	-	-	-	-
14.88	?	?	-	-	-	-	-
15.24	49	2,4-dimethylpentane	30.6	0.0	0.0	0.0	0.0
15.29	?	?	-	-	-	-	-
15.48	?	?	-	-	-	-	-
15.69	?	?	-	-	-	-	-
15.88	52	benzene	0.0	0.0	13.6	0.0	0.0
16.1	54	cyclohexane	12.8	0.0	0.0	0.0	0.0
16.22	55	2-methylhexane	15.7	0.0	0.0	0.0	0.0
16.3	56	2,3-dimethylpentane	20.4	0.0	0.0	0.0	0.0
16.45	57	3-methylhexane	20.6	0.0	0.0	0.0	0.0
16.79	58	2,2,4-trimethylpentane	19.9	0.0	0.0	0.0	0.0
16.95	59	ISTD 2	-	-	-	-	-
17.31	?	?	-	-	-	-	-

17.63	63	methylcyclohexane/MIBK	17.7	0.0	0.0	0.0	0.0
17.83	?	?	-	-	-	-	-
18.2	64	1,1,2-trichloroethane	-	-	-	-	-
18.3	65	2,3,4-trimethylpentane	15.8	0.0	0.0	0.0	0.0
18.48	66	toluene	0.0	0.0	13.6	0.0	0.0
18.61	67	2-methylheptane	17.0	0.0	0.0	0.0	0.0
18.72	?	?	-	-	-	-	-
18.82	68	3-methylheptane	16.9	0.0	0.0	0.0	0.0
18.97	69	hexanal	-	-	-	-	-
19.46	70	n-octane	16.1	0.0	0.0	0.0	0.0
20.36	?	?	-	-	-	-	-
20.99	71	ethylbenzene	0.0	0.0	15.4	0.0	0.0
21.23	72	p-xylene & m-xylene	0.0	0.0	28.6	0.0	0.0
21.43	?	?	-	-	-	-	-
21.7	75	styrene	0.0	0.0	94.1	0.0	0.0
21.9	76	o-xylene	0.0	0.0	13.5	0.0	0.0
22.17	77	n-nonane	21.6	0.0	0.0	0.0	0.0
22.6	78	ISTD 3	-	-	-	-	-
22.82	79	isopropylbenzene	0.0	0.0	16.6	0.0	0.0
23.32	?	?	-	-	-	-	-
23.49	81	benzaldehyde/alpha-pinene	0.0	0.0	0.0	19.3	0.0
23.72	83	n-propylbenzene	0.0	0.0	22.0	0.0	0.0
24.14	85	1,3,5-trimethylbenzene	0.0	0.0	16.5	0.0	0.0
24.83	88	beta-pinene	-	-	-	-	-
24.98	89	1,2,4-trimethylbenzene	0.0	0.0	17.9	0.0	0.0
26.79	95	m-diethylbenzene	-	-	-	-	-
30.29	?	?	-	-	-	-	-
			512.8	29.7	251.9	73.6	30.3

Peak Report -- Channel A

36173			RT (min)
0.586		ISTD 1	7.827
Smog Chamber		ISTD 2	16.933
c:\sarah\3-2		ISTD 3	22.577
c:\ezchrom\methods\0to15.met			
System Peaks	52		

RT (min)	Peak ID	Compound	Area	Height	Area of Knowns	Area of Unknowns	Conc (ppbv)	ppbC
6.517	5	propane	7233	2407	7233	-	1.1	3.2
6.597	?	?	10828	3609	-	10828	-	-
7.827	9	ISTD 1	197591	59777	-	-	-	-
8.26	11b	1,3-butadiene	14947	3493	14947	-	0.9	3.6
8.423	?	?	9709	2375	-	9709	-	-
8.667	?	?	16003	5674	-	16003	-	-
10.42	?	?	9198	1678	-	9198	-	-
10.65	20b	2-propenal	13779	4768	13779	-	4.3	12.9
10.84	21	isopentane	28090	12791	28090	-	2.7	13.3
10.9	21	isopentane	157979	40454	157979	-	14.9	74.7
11.63	?	?	15240	6240	-	15240	-	-
12.67	?	?	22291	8486	-	22291	-	-
12.89	31	cyclopentene	10577	3649	10577	-	0.8	3.9
13.21	?	?	6771	2361	-	6771	-	-
13.27	?	?	6340	2258	-	6340	-	-
13.48	23	1-pentene	14785	6467	14785	-	1.5	7.3
13.52	37	2-methylpentane	21637	8336	21637	-	1.5	7.4
13.64	40	butanal	33550	11628	33550	-	6.0	23.9
13.76	40b	2-butanone	39569	13628	39569	-	6.5	26.1
14.03	?	?	38093	10174	-	38093	-	-
14.48	44	n-hexane	17081	7596	17081	-	1.2	7.2
15.22	49	2,4-dimethylpentane	15753	6517	15753	-	1.0	6.7
15.28	?	?	29087	9105	-	29087	-	-
15.48	?	?	7191	1786	-	7191	-	-
15.75	?	?	7176	1568	-	7176	-	-
15.86	52	benzene	30924	12083	30924	-	2.3	13.7
16.09	54	cyclohexane	18440	6896	18440	-	1.3	8.0
16.21	55	2-methylhexane	27699	11793	27699	-	1.7	12.1
16.28	56	2,3-dimethylpentane	17388	7591	17388	-	1.1	7.7
16.37	57	3-methylhexane	5565	2626	5565	-	0.3	1.9
16.43	57	3-methylhexane	5930	3709	5930	-	0.3	2.1
16.78	58	2,2,4-trimethylpentane	25452	10455	25452	-	1.6	12.9
16.93	59	ISTD 2	270179	108014	-	-	-	-
17.29	?	?	8094	2997	-	8094	-	-
17.61	63	methylcyclohexane/MIBK	19401	5897	19401	-	1.2	8.7
18.28	65	2,3,4-trimethylpentane	22491	7489	22491	-	1.5	11.7
18.45	66	toluene	29216	9631	29216	-	1.9	13.5
18.59	67	2-methylheptane	17999	6867	17999	-	1.1	9.1
18.8	68	3-methylheptane	24662	7184	24662	-	1.6	12.8
18.97	69	hexanal	8740	2804	8740	-	1.3	8.1
19.44	70	n-octane	16506	6166	16506	-	0.9	7.6
20.97	71	ethylbenzene	21787	6983	21787	-	1.3	10.0
21.21	72	p-xylene & m-xylene	24941	6077	24941	-	1.7	13.7
21.88	76	o-xylene	14395	4382	14395	-	1.0	8.2

22.14	77	n-nonane	20751	5352	20751	-	1.2	10.6
22.58	78	ISTD 3	30959	8734	-	-	-	-
22.79	79	isopropylbenzene	18979	5726	18979	-	1.6	14.2
23.69	83	n-propylbenzene	19393	5093	19393	-	1.6	14.8
26.35	?	?	5247	365	-	5247	-	-
28	?	?	5049	768	-	5049	-	-
30.57	?	?	6936	381	-	6936	-	-
32.09	?	?	6693	557	-	6693	-	-
					765639	209946	68.9	391.6

Total Area	975585
Area of Knowns	765639
Area of Unknowns	209946
Total Area/Known Area	1.274
Known ppbC	392
Total ppbC	499

Peak Report -- Channel A
36173
0.586
Smog
Chamber
c:\sarah\3-2
c:\ezchrom\methods\0to15.met
System
Peaks

RT (min)	Peak ID	Compound	Paraffin (ppbC)	Olefin (ppbC)	Aromatic (ppbC)	Carbonyl (ppbC)	Alcohol (ppbC)
6.517	5	propane	3.2	0.0	0.0	0.0	0.0
6.597	?	?	-	-	-	-	-
7.827	9	ISTD 1	-	-	-	-	-
8.26	11b	1,3-butadiene	-	-	-	-	-
8.423	?	?	-	-	-	-	-
8.667	?	?	-	-	-	-	-
10.42	?	?	-	-	-	-	-
10.65	20b	2-propenal	0.0	0.0	0.0	12.9	0.0
10.84	21	isopentane	13.3	0.0	0.0	0.0	0.0
10.9	21	isopentane	74.7	0.0	0.0	0.0	0.0
11.63	?	?	-	-	-	-	-
12.67	?	?	-	-	-	-	-
12.89	31	cyclopentene	-	-	-	-	-
13.21	?	?	-	-	-	-	-
13.27	?	?	-	-	-	-	-
13.48	23	1-pentene	0.0	7.3	0.0	0.0	0.0
13.52	37	2-methylpentane	7.4	0.0	0.0	0.0	0.0
13.64	40	butanal	0.0	0.0	0.0	23.9	0.0
13.76	40b	2-butanone	0.0	0.0	0.0	26.1	0.0
14.03	?	?	-	-	-	-	-
14.48	44	n-hexane	7.2	0.0	0.0	0.0	0.0
15.22	49	2,4-dimethylpentane	6.7	0.0	0.0	0.0	0.0
15.28	?	?	-	-	-	-	-
15.48	?	?	-	-	-	-	-
15.75	?	?	-	-	-	-	-
15.86	52	benzene	0.0	0.0	13.7	0.0	0.0
16.09	54	cyclohexane	8.0	0.0	0.0	0.0	0.0
16.21	55	2-methylhexane	12.1	0.0	0.0	0.0	0.0
16.28	56	2,3-dimethylpentane	7.7	0.0	0.0	0.0	0.0
16.37	57	3-methylhexane	1.9	0.0	0.0	0.0	0.0
16.43	57	3-methylhexane	2.1	0.0	0.0	0.0	0.0
16.78	58	2,2,4-trimethylpentane	12.9	0.0	0.0	0.0	0.0
16.93	59	ISTD 2	-	-	-	-	-
17.29	?	?	-	-	-	-	-
17.61	63	methylcyclohexane/MIBK	8.7	0.0	0.0	0.0	0.0
18.28	65	2,3,4-trimethylpentane	11.7	0.0	0.0	0.0	0.0
18.45	66	toluene	0.0	0.0	13.5	0.0	0.0
18.59	67	2-methylheptane	9.1	0.0	0.0	0.0	0.0
18.8	68	3-methylheptane	12.8	0.0	0.0	0.0	0.0
18.97	69	hexanal	-	-	-	-	-
19.44	70	n-octane	7.6	0.0	0.0	0.0	0.0
20.97	71	ethylbenzene	0.0	0.0	10.0	0.0	0.0
21.21	72	p-xylene & m-xylene	0.0	0.0	13.7	0.0	0.0
21.88	76	o-xylene	0.0	0.0	8.2	0.0	0.0

22.14	77	n-nonane	10.6	0.0	0.0	0.0	0.0
22.58	78	ISTD 3	-	-	-	-	-
22.79	79	isopropylbenzene	0.0	0.0	14.2	0.0	0.0
23.69	83	n-propylbenzene	0.0	0.0	14.8	0.0	0.0
26.35	?	?	-	-	-	-	-
28	?	?	-	-	-	-	-
30.57	?	?	-	-	-	-	-
32.09	?	?	-	-	-	-	-
			217.7	7.3	88.2	62.9	0.0

Peak Report -- Channel A

36264		RT (min)	
0.982	ISTD 1	8.15	
smog chamber	ISTD 2	17.217	
c:\sarah\sc4-1	ISTD 3	22.958	
c:\ezchrom\methods\0to15.met			
System			
Peaks 57			

RT (min)	Peak ID	Compound	Area	Height	Area of Knowns	Area of Unknowns	Conc (ppbv)	ppbC
6.8	5	propane	15804	4912	15804	-	2.3	6.9
6.883	?	?	10523	3173	-	10523	-	-
8.15	9	ISTD 1	76998	18141	-	-	-	-
8.6	12	n-butane	3086	930	3086	-	0.4	1.4
8.733	?	?	20735	6301	-	20735	-	-
8.967	?	?	17312	5952	-	17312	-	-
9.267	14	bromomethane	17058	5836	17058	-	7.9	7.9
9.675	?	?	15437	5374	-	15437	-	-
10.61	19	ethanol	21617	7841	21617	-	9.2	18.5
10.98	20b	2-propenal	3246	492	3246	-	1.0	3.0
11.13	21	isopentane	39271	14423	39271	-	3.7	18.6
11.25	22b	acetone/propanal	43845	9577	43845	-	18.3	55.0
11.58	?	?	20865	7783	-	20865	-	-
11.92	?	?	19696	7517	-	19696	-	-
12.07	25	isoprene	16049	6000	16049	-	1.6	8.0
12.16	?	?	19399	7644	-	19399	-	-
12.38	26	trans-2-pentene	18408	7047	18408	-	1.8	9.2
12.53	?	?	15105	5794	-	15105	-	-
12.96	?	?	23050	8660	-	23050	-	-
13.2	31	cyclopentene	1318	420	1318	-	0.1	0.5
13.47	?	?	18897	6958	-	18897	-	-
13.56	23	1-pentene	26434	9383	26434	-	2.6	13.0
13.81	?	?	42215	9510	-	42215	-	-
13.93	40	butanal	24836	9543	24836	-	4.4	17.7
14.08	40b	2-butanone	3195	886	3195	-	0.5	2.1
14.32	43	2-methyl-1-pentene	21274	8338	21274	-	12.0	72.0
14.45	?	?	20166	7125	-	20166	-	-
14.77	44	n-hexane	24746	9875	24746	-	1.7	10.4
14.89	?	?	20437	8457	-	20437	-	-
15.14	?	?	20560	8345	-	20560	-	-
15.56	?	?	50034	11040	-	50034	-	-
16.14	52	benzene	24225	9008	24225	-	1.8	10.7
16.38	?	?	23130	8673	-	23130	-	-
16.48	55	2-methylhexane	30137	12180	30137	-	1.9	13.1
16.56	56	2,3-dimethylpentane	26010	10203	26010	-	1.6	11.5
16.71	57	3-methylhexane	27809	10889	27809	-	1.4	9.7
17.06	58	2,2,4-trimethylpentane	30164	11900	30164	-	1.9	15.3
17.22	59	ISTD 2	3E+05	121783	-	-	-	-
17.92	63	methylcyclohexane/MIBK	24720	8851	24720	-	1.6	11.1
18.6	65	2,3,4-trimethylpentane	27620	9983	27620	-	1.8	14.4
18.78	66	toluene	25898	8626	25898	-	1.7	12.0
18.91	67	2-methylheptane	28011	10251	28011	-	1.8	14.1
19.13	68	3-methylheptane	28695	10016	28695	-	1.9	14.9
19.78	70	n-octane	28550	10384	28550	-	1.6	13.1

21.33	71	ethylbenzene	23707	7385	23707	-	1.4	10.9
21.57	72	p-xylene & m-xylene	46733	10474	46733	-	3.2	25.8
22.08	75	styrene	992	305	992	-	0.3	2.2
22.25	76	o-xylene	20559	6177	20559	-	1.5	11.8
22.51	77	n-nonane	42031	11001	42031	-	2.4	21.5
22.96	78	ISTD 3	1E+05	33889	-	-	-	-
23.18	79	isopropylbenzene	18991	5513	18991	-	1.6	14.2
24.08	83	n-propylbenzene	22742	5968	22742	-	1.9	17.3
24.52	85	1,3,5-trimethylbenzene	1905	593	1905	-	0.2	1.8
24.89	86	o-ethyltoluene	5148	466	5148	-	0.5	4.7
25.36	89	1,2,4-trimethylbenzene	5204	1457	5204	-	0.6	5.3
28.44	?	?	1313	383	-	1313	-	-
28.93	?	?	1204	251	-	1204	-	-
					770038	360078	100.2	499.8

Total Area	1E+06
Area of Knowns	8E+05
Area of Unknowns	4E+05
Total Area/Known Area	1.468
Known ppbC	500
Total ppbC	733

Peak Report -- Channel A
36264
0.982
smog chamber
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c:\ezchrom\methods\0to15.met
System
Peaks

RT (min)	Peak ID	Compound	Paraffin (ppbC)	Olefin (ppbC)	Aromatic (ppbC)	Carbonyl (ppbC)	Alcohol (ppbC)
6.8	5	propane	6.9	0.0	0.0	0.0	0.0
6.883	?	?	-	-	-	-	-
8.15	9	ISTD 1	-	-	-	-	-
8.6	12	n-butane	1.4	0.0	0.0	0.0	0.0
8.733	?	?	-	-	-	-	-
8.967	?	?	-	-	-	-	-
9.267	14	bromomethane	-	-	-	-	-
9.675	?	?	-	-	-	-	-
10.61	19	ethanol	0.0	0.0	0.0	0.0	18.5
10.98	20b	2-propenal	0.0	0.0	0.0	3.0	0.0
11.13	21	isopentane	18.6	0.0	0.0	0.0	0.0
11.25	22b	acetone/propanal	0.0	0.0	0.0	55.0	0.0
11.58	?	?	-	-	-	-	-
11.92	?	?	-	-	-	-	-
12.07	25	isoprene	0.0	8.0	0.0	0.0	0.0
12.16	?	?	-	-	-	-	-
12.38	26	trans-2-pentene	0.0	9.2	0.0	0.0	0.0
12.53	?	?	-	-	-	-	-
12.96	?	?	-	-	-	-	-
13.2	31	cyclopentene	-	-	-	-	-
13.47	?	?	-	-	-	-	-
13.56	23	1-pentene	0.0	13.0	0.0	0.0	0.0
13.81	?	?	-	-	-	-	-
13.93	40	butanal	0.0	0.0	0.0	17.7	0.0
14.08	40b	2-butanone	0.0	0.0	0.0	2.1	0.0
14.32	43	2-methyl-1-pentene	0.0	72.0	0.0	0.0	0.0
14.45	?	?	-	-	-	-	-
14.77	44	n-hexane	10.4	0.0	0.0	0.0	0.0
14.89	?	?	-	-	-	-	-
15.14	?	?	-	-	-	-	-
15.56	?	?	-	-	-	-	-
16.14	52	benzene	0.0	0.0	10.7	0.0	0.0
16.38	?	?	-	-	-	-	-
16.48	55	2-methylhexane	13.1	0.0	0.0	0.0	0.0
16.56	56	2,3-dimethylpentane	11.5	0.0	0.0	0.0	0.0
16.71	57	3-methylhexane	9.7	0.0	0.0	0.0	0.0
17.06	58	2,2,4-trimethylpentane	15.3	0.0	0.0	0.0	0.0
17.22	59	ISTD 2	-	-	-	-	-
17.92	63	methylcyclohexane/MIBK	11.1	0.0	0.0	0.0	0.0
18.6	65	2,3,4-trimethylpentane	14.4	0.0	0.0	0.0	0.0
18.78	66	toluene	0.0	0.0	12.0	0.0	0.0
18.91	67	2-methylheptane	14.1	0.0	0.0	0.0	0.0
19.13	68	3-methylheptane	14.9	0.0	0.0	0.0	0.0
19.78	70	n-octane	13.1	0.0	0.0	0.0	0.0
21.33	71	ethylbenzene	0.0	0.0	10.9	0.0	0.0

21.57	72	p-xylene & m-xylene	0.0	0.0	25.8	0.0	0.0
22.08	75	styrene	0.0	0.0	2.2	0.0	0.0
22.25	76	o-xylene	0.0	0.0	11.8	0.0	0.0
22.51	77	n-nonane	21.5	0.0	0.0	0.0	0.0
22.96	78	ISTD 3	-	-	-	-	-
23.18	79	isopropylbenzene	0.0	0.0	14.2	0.0	0.0
24.08	83	n-propylbenzene	0.0	0.0	17.3	0.0	0.0
24.52	85	1,3,5-trimethylbenzene	0.0	0.0	1.8	0.0	0.0
24.89	86	o-ethyltoluene	-	-	-	-	-
25.36	89	1,2,4-trimethylbenzene	0.0	0.0	5.3	0.0	0.0
28.44	?	?	-	-	-	-	-
28.93	?	?	-	-	-	-	-
			176.1	102.1	112.0	77.9	18.5

Peak Report -- Channel A

36264		RT (min)	
0.837	ISTD 1	8	
smog chamber	ISTD 2	17.083	
c:\sarah\sc4-2	ISTD 3	22.783	
c:\ezchrom\methods\0to15.met			
System Peaks	64		

RT (min)	Peak ID	Compound	Area	Height	Area of Knowns	Area of Unknowns	Conc (ppbv)	ppbC
5.983	?	?	3875	1400	-	3875	-	-
6.667	5	propane	12342	3843	12342	-	1.8	5.4
6.742	?	?	10042	3212	-	10042	-	-
8	9	ISTD 1	115845	31880	-	-	-	-
8.442	12	n-butane	5847	1586	5847	-	0.7	2.7
8.592	?	?	13699	3926	-	13699	-	-
8.833	?	?	17609	6167	-	17609	-	-
9.133	14	bromomethane	2487	818	2487	-	1.2	1.2
9.533	?	?	3127	984	-	3127	-	-
10.48	19	ethanol	10915	4040	10915	-	4.7	9.3
10.65	?	?	3273	616	-	3273	-	-
10.83	20b	2-propenal	4955	1644	4955	-	1.5	4.6
11	21	isopentane	37641	14309	37641	-	3.6	17.8
11.09	22b	acetone/propanal	81946	20189	81946	-	34.3	102.8
11.45	?	?	11244	4225	-	11244	-	-
11.78	?	?	19170	7488	-	19170	-	-
11.93	24	n-pentane	1804	669	1804	-	0.2	0.8
12.03	25	isoprene	2298	896	2298	-	0.2	1.1
12.25	26b	1,1-dichloroethylene	2999	1142	2999	-	0.6	1.2
12.83	?	?	23508	8830	-	23508	-	-
13.05	31	cyclopentene	3670	1248	3670	-	0.3	1.3
13.43	23	1-pentene	17746	5032	17746	-	1.8	8.8
13.68	37	2-methylpentane	40531	8949	40531	-	2.8	13.9
13.79	40	butanal	23702	9366	23702	-	4.2	16.9
13.93	40b	2-butanone	17706	5186	17706	-	2.9	11.7
14.18	43	2-methyl-1-pentene	25132	8355	25132	-	14.2	85.0
14.32	?	?	6429	2142	-	6429	-	-
14.63	44	n-hexane	23982	9477	23982	-	1.7	10.1
14.76	?	?	3571	1234	-	3571	-	-
15.01	?	?	4028	1370	-	4028	-	-
15.43	?	?	46904	10564	-	46904	-	-
15.66	?	?	5776	638	-	5776	-	-
16.01	52	benzene	26017	9297	26017	-	1.9	11.5
16.23	52	benzene	20765	7757	20765	-	1.5	9.2
16.35	55	2-methylhexane	30752	12367	30752	-	1.9	13.4
16.43	56	2,3-dimethylpentane	22933	9246	22933	-	1.4	10.1
16.58	57	3-methylhexane	32466	11219	32466	-	1.6	11.4
16.93	58	2,2,4-trimethylpentane	32290	11943	32290	-	2.0	16.4
17.08	59	ISTD 2	341685	128831	-	-	-	-
17.45	?	?	1242	508	-	1242	-	-
17.78	63	methylcyclohexane/MIBK	22326	7593	22326	-	1.4	10.0
18.45	65	2,3,4-trimethylpentane	24441	8982	24441	-	1.6	12.8
18.63	66	toluene	24236	8253	24236	-	1.6	11.2

18.76	67	2-methylheptane	24338	8848	24338	-	1.5	12.3
18.98	68	3-methylheptane	24554	8428	24554	-	1.6	12.7
19.17	69	hexanal	2500	404	2500	-	0.4	2.3
19.33	?	?	1726	474	-	1726	-	-
19.62	70	n-octane	26135	9057	26135	-	1.5	12.0
20.13	?	?	16845	1615	-	16845	-	-
21.16	71	ethylbenzene	20458	6540	20458	-	1.2	9.4
21.4	72	p-xylene & m-xylene	30258	7243	30258	-	2.1	16.7
21.92	75	styrene	1576	455	1576	-	0.4	3.6
22.08	76	o-xylene	15971	4838	15971	-	1.1	9.1
22.34	77	n-nonane	42633	11234	42633	-	2.4	21.8
22.78	78	ISTD 3	104321	30943	-	-	-	-
23	79	isopropylbenzene	18092	5420	18092	-	1.5	13.5
23.68	81	benzaldehyde/alpha-pinene	1487	452	1487	-	0.1	0.7
23.91	83	n-propylbenzene	20975	5453	20975	-	1.8	16.0
24.33	85	1,3,5-trimethylbenzene	2012	642	2012	-	0.2	1.9
25.18	89	1,2,4-trimethylbenzene	5328	1577	5328	-	0.6	5.4
25.92	?	?	1063	257	-	1063	-	-
27.01	95	m-diethylbenzene	2275	288	2275	-	0.4	4.2
28.25	?	?	736	264	-	736	-	-
28.88	98	n-undecane	7588	989	7588	-	0.6	6.8
					798109	193867	109.1	549.1

Total Area	991976
Area of Knowns	798109
Area of Unknowns	193867
Total Area/Known Area	1.243
Known ppbC	549
Total ppbC	683

Peak Report -- Channel A
36264
0.837
smog chamber
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Peaks

RT (min)	Peak ID	Compound	Paraffin (ppbC)	Olefin (ppbC)	Aromatic (ppbC)	Carbonyl (ppbC)	Alcohol (ppbC)
5.983	?	?	-	-	-	-	-
6.667	5	propane	5.4	0.0	0.0	0.0	0.0
6.742	?	?	-	-	-	-	-
8	9	ISTD 1	-	-	-	-	-
8.442	12	n-butane	2.7	0.0	0.0	0.0	0.0
8.592	?	?	-	-	-	-	-
8.833	?	?	-	-	-	-	-
9.133	14	bromomethane	-	-	-	-	-
9.533	?	?	-	-	-	-	-
10.48	19	ethanol	0.0	0.0	0.0	0.0	9.3
10.65	?	?	-	-	-	-	-
10.83	20b	2-propenal	0.0	0.0	0.0	4.6	0.0
11	21	isopentane	17.8	0.0	0.0	0.0	0.0
11.09	22b	acetone/propanal	0.0	0.0	0.0	102.8	0.0
11.45	?	?	-	-	-	-	-
11.78	?	?	-	-	-	-	-
11.93	24	n-pentane	0.8	0.0	0.0	0.0	0.0
12.03	25	isoprene	0.0	1.1	0.0	0.0	0.0
12.25	26b	1,1-dichloroethylene	-	-	-	-	-
12.83	?	?	-	-	-	-	-
13.05	31	cyclopentene	-	-	-	-	-
13.43	23	1-pentene	0.0	8.8	0.0	0.0	0.0
13.68	37	2-methylpentane	13.9	0.0	0.0	0.0	0.0
13.79	40	butanal	0.0	0.0	0.0	16.9	0.0
13.93	40b	2-butanone	0.0	0.0	0.0	11.7	0.0
14.18	43	2-methyl-1-pentene	0.0	85.0	0.0	0.0	0.0
14.32	?	?	-	-	-	-	-
14.63	44	n-hexane	10.1	0.0	0.0	0.0	0.0
14.76	?	?	-	-	-	-	-
15.01	?	?	-	-	-	-	-
15.43	?	?	-	-	-	-	-
15.66	?	?	-	-	-	-	-
16.01	?	?	0.0	0.0	11.5	0.0	0.0
16.23	52	benzene	0.0	0.0	9.2	0.0	0.0
16.35	55	2-methylhexane	13.4	0.0	0.0	0.0	0.0
16.43	56	2,3-dimethylpentane	10.1	0.0	0.0	0.0	0.0
16.58	57	3-methylhexane	11.4	0.0	0.0	0.0	0.0
16.93	58	2,2,4-trimethylpentane	16.4	0.0	0.0	0.0	0.0
17.08	59	ISTD 2	-	-	-	-	-
17.45	?	?	-	-	-	-	-
17.78	63	methylcyclohexane/MIBK	10.0	0.0	0.0	0.0	0.0
18.45	65	2,3,4-trimethylpentane	12.8	0.0	0.0	0.0	0.0
18.63	66	toluene	0.0	0.0	11.2	0.0	0.0
18.76	67	2-methylheptane	12.3	0.0	0.0	0.0	0.0

18.98	68	3-methylheptane	12.7	0.0	0.0	0.0	0.0
19.17	69	hexanal	-	-	-	-	-
19.33	?	?	-	-	-	-	-
19.62	70	n-octane	12.0	0.0	0.0	0.0	0.0
20.13	?	?	-	-	-	-	-
21.16	71	ethylbenzene	0.0	0.0	9.4	0.0	0.0
21.4	72	p-xylene & m-xylene	0.0	0.0	16.7	0.0	0.0
21.92	75	styrene	0.0	0.0	3.6	0.0	0.0
22.08	76	o-xylene	0.0	0.0	9.1	0.0	0.0
22.34	77	n-nonane	21.8	0.0	0.0	0.0	0.0
22.78	78	ISTD 3	-	-	-	-	-
23	79	isopropylbenzene	0.0	0.0	13.5	0.0	0.0
23.68	81	benzaldehyde/alpha-pinene	0.0	0.0	0.0	0.7	0.0
23.91	83	n-propylbenzene	0.0	0.0	16.0	0.0	0.0
24.33	85	1,3,5-trimethylbenzene	0.0	0.0	1.9	0.0	0.0
25.18	89	1,2,4-trimethylbenzene	0.0	0.0	5.4	0.0	0.0
25.92	?	?	-	-	-	-	-
27.01	95	m-diethylbenzene	-	-	-	-	-
28.25	?	?	-	-	-	-	-
28.88	98	n-undecane	6.8	0.0	0.0	0.0	0.0
			190.4	94.9	107.6	136.7	9.3

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