Aerosol Formation from Atmospheric Hydrocarbon Photooxidation

Thesis by
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ABSTRACT

Outdoor smog chamber experiments have been performed to determine the secondary organic aerosol (SOA) formation potential of various C_7, C_8, and C_9 aromatics in sunlight-irradiated hydrocarbon-NO_X mixtures. Measured aerosol yields from toluene, *m*-xylene, *p*-xylene, ethylbenzene, *m*-ethyltoluene, *p*-ethyltoluene, and 1,2,4-trimethylbenzene were found to correlate with organic mass concentration according to semi-volatile gas/particle partitioning theory. Aerosol yields of the C_9 aromatics were greater than those of the C_8 aromatics, with *m*-ethyltoluene resulting in the greatest yields. Toluene and ethylbenzene demonstrated some aerosol-forming potential, but the other aromatics produced significantly more SOA.

Filter samples were also collected during the experiments to determine the molecular composition of the SOA from these aromatics Gas-phase mechanisms leading to these products have been proposed. Unsaturated anhydrides (2,5-furandione, 3-methyl-2,5-furandione, 3-ethyl-2,5-furandione) are predominant components of aerosol from all the aromatics, an observation that is consistent with gas-phase aromatic mechanisms involving ring-fragmentation. Saturated anhydrides were also detected in significant quantities, which could result from the hydrogenation of furandiones in sunlight in the particle phase. A new organic aerosol extraction procedure utilizing supercritical CO_2 extraction is outlined.

Outdoor smog chamber experiments were also performed to characterize aerosol from 1-octene and 1-decene photooxidation. The dominant aerosol species were heptanal, heptanoic acid, and dihydro-5-propyl-2(3H)-furanone from 1-octene, and nonanal, nonanoic acid, and dihydro-5-pentyl-2(3H)-furanone from 1-decene. Gas-phase oxidation mechanisms of 1-octene and 1-decene with OH and O_3 account for the aerosol products.

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CHAPTER 1

Introduction

Sources of Air Pollution

Urban air pollution is a complex mixture of gaseous and particulate components which originate from the emissions of inorganic and organic compounds from anthropogenic and biogenic sources, and from the chemical interactions of these compounds once emitted. Primary pollutants are those emitted directly from sources. Secondary pollutants are formed from the chemical transformations of primary pollutants. In urban atmospheres, photochemical smog formation and the associated high ozone levels continue to be the most pervasive problems despite major regulatory and pollution-control efforts. Photochemical smog is the mixture of reactants and products involved in a complex series of reactions occurring in sunlight between emitted nitrogen oxides (NO_X) and volatile organic compounds (VOCs) (Seinfeld, 1986; Seinfeld, 1989; Seinfeld *et al.*, 1994).

Sources of primary pollutants have been well-established in recent years with the establishment of the National Emissions Data System in 1971 by the U.S. Environmental Protection Agency (National Research Council, 1991). Major sources of VOCs have been identified: vegetation, motor vehicle exhaust, emissions from commercial and industrial solvents, and fugitive emissions from chemical and petroleum industries. Motor vehicle exhausts and stationary combustion system exhausts (*i.e.,* electric power generation, industrial and domestic fuel burning) were identified as important NO_X sources (National Research Council, 1991; Seinfeld, 1986). Figures 1.1 and 1.2 identify sources of NO_X and VOCs according to the 1985 national emissions inventory. In addition to identifying sources of gaseous pollutants, recent work has been done to apportion sources of particulate matter. With reference to the Los Angeles basin, Rogge *et al.* (1991, 1993abcd) have identified major sources of primary organic aerosol: charbroilers and other meat

cooking operations, automobiles and heavy-duty diesel trucks, road dust, tire debris, brake lining dust, particulates from leaf surfaces, and natural gas home appliances.

In addition to identifying emission sources for gaseous and particulate components, our knowledge of the composition of urban atmospheres is also well-established. A comprehensive field study was carried out in 1987 in the South Coast Air Basin, which experiences the most severe air pollution in the U.S. During this study, the Southern California Air Quality Study (SCAQS), meteorological parameters, gaseous inorganic and organic species, and aerosols were monitored for 11 days during the summer and six days during the fall. The meteorological parameters measured included inversion height, temperature, dew point, and wind speed and direction. The gaseous inorganic species monitored were hydrogen peroxide, nitric oxide, nitrogen dioxide, ozone, carbon monoxide, sulfur dioxide, nitrous acid, and nitric acid. The organic species monitored were RO radicals, organic acids, aldehydes, ketones, alcohols, C_1-C_{12} hydrocarbons, and peroxyacetyl nitrate. Aerosol measurements included physical size distributions, light scattering, PM-10 mass, and measurements of aerosol composition, such as sulfate ion, ammonium ion, nitrate ion, chloride ion, organic carbon, elemental carbon, and black carbon (Lawson, 1990).

Studies have been conducted on particulate matter, to determine the concentrations and composition of urban aerosols. Heintzenberg (1989) compiled 21 urban aerosol data sets from the U.S., Japan, U.K., Germany, China, Sweden and Brazil to arrive at a global, average urban fine (less than 1 μm radius) particle composition, shown in Figure 1.3. Solomon *et al.* (1989) also determined the aerosol composition at several locations in the South Coast Air Basin in 1986. The ambient aerosol composition of samples from downtown Los Angeles and Anaheim are shown in Figure 1.4. Urban aerosol in the Los Angeles basin was shown to consist of a significant fraction of organic species which arise from primary emissions and secondary processes in the atmosphere.

With emissions inventories and field studies, the nature of primary pollutants is well understood. However, the chemical and associated physical processes transforming primary pollutants after their release into the atmosphere is much more complex and areas of uncertainty exist in our understanding of them.

Secondary Processes in Urban Atmosphere - Gas-to-Particle Conversion

The emission of volatile organic compounds and nitrogen oxides leads to a complex array of reactions in the gas-phase. The chemistry of these species with themselves and other natural constituents of the atmosphere has received intense study (Atkinson, 1994; National Research Council, 1991; Seinfeld, 1986; Seinfeld *et al.*, 1994; and references therein). Rather than attempting to review the chemistry of all classes of compounds in the atmosphere, the chemistry pertaining to the formation of secondary aerosol will be discussed.

Volatile organic compounds found in urban atmospheres include alkanes, alkenes, aromatics, biogenic species such as terpenes and sesquiterpenes, and oxygen-containing compounds such as carbonyls (aldehydes, ketones, organic acids), ethers, and alcohols. Table 1.1 lists the non-methane organic compounds measured during SCAQS ordered with respect to percentage of the total non-methane organic compound concentration on a carbon basis. The VOCs were determined to be 45% alkanes, 9% alkenes, 18% aromatics, 13% carbonyl compounds, with the remainder unidentified (Lurmann and Main, 1992). In the presence of sunlight, these hydrocarbons react in the gas-phase with hydroxyl radicals, nitrate radicals and ozone which are present in the urban atmosphere to yield oxygenated and nitrated products. These reaction products are often less volatile than the original hydrocarbons, and may condense onto the particle phase. This gas-to-particle conversion process, outlined in Figure 1.5, involves condensation of the products onto exisiting particles, or nucleation to form ultra-fine particles. This resulting aerosol is referred to as

secondary organic aerosol (SOA), and partly comprises the organic fraction of urban aerosol along with primary emissions, as depicted in Figures 1.3 and 1.4. The relative contribution of secondary organic aerosol to this organic fraction has been estimated to be as much as 70% (Turpin and Huntzicker, 1991). Clearly, gas-to-particle conversion plays an important role in the urban atmosphere.

Quantifying aerosol formation from the photooxidation of hydrocarbon precursors has until now largely involved the measurement of aerosol yield, defined as the ratio of secondary aerosol produced (in terms of volume or mass concentration) to the amount of hydrocarbon reacted. Smog chamber studies have historically provided yield data by measuring secondary organic aerosol produced from the photooxidation of a hydrocarbon in the presence of nitrogen oxides in a controlled environment. One goal of these studies was to estimate the contribution of SOA to the total ambient aerosol based on these yields. Table 1.2 summarizes reported aerosol yields of hydrocarbons. Upon considering Table 1.2, it becomes apparent that although numerous hydrocarbons are aerosol precurors, few studies have identified the components of SOA. This information is critical in understanding gas-to-particle conversion processes, as well as the gas-phase photooxidation chemistry associated with the parent hydrocarbon.

Research Objectives

The motivation for this research stems from the lack of information on composition of secondary organic aerosol. A number of organics were investigated to determine whether or not each organic produces SOA, to identify species in the SOA formed from each precursor, and to determine to the extent possible the gas-phase oxidation mechanisms leading to SOA. The organics were selected based on their predominance in SCAQS (Lurmann and Main, 1992). The aromatics studied were toluene, *m*-xylene, *p*-xylene, ethylbenzene, *m*-ethyltoluene, *p*-ethyltoluene, and 1,2,4-trimethylbenzene. The first part of this thesis describes a series of outdoor smog chamber experiments to measure the secondary organic aerosol yields from the photooxidation of the seven aromatics in the presence of nitrogen oxides. The second part of this thesis describes the composition of the SOA samples collected from the aforementioned aromatic experiments. In addition to listing the reaction products identified in the particle phase, gas-phase mechanisms leading to these products are proposed. The third part of this thesis describes more smog chamber experiments of the photooxidation of octene and decene and the analysis of SOA. Again, gas-phase mechanisms leading to the products identified in the octene and decene SOA are proposed. Finally, the development of the technique used to prepare the aerosol samples is outlined.

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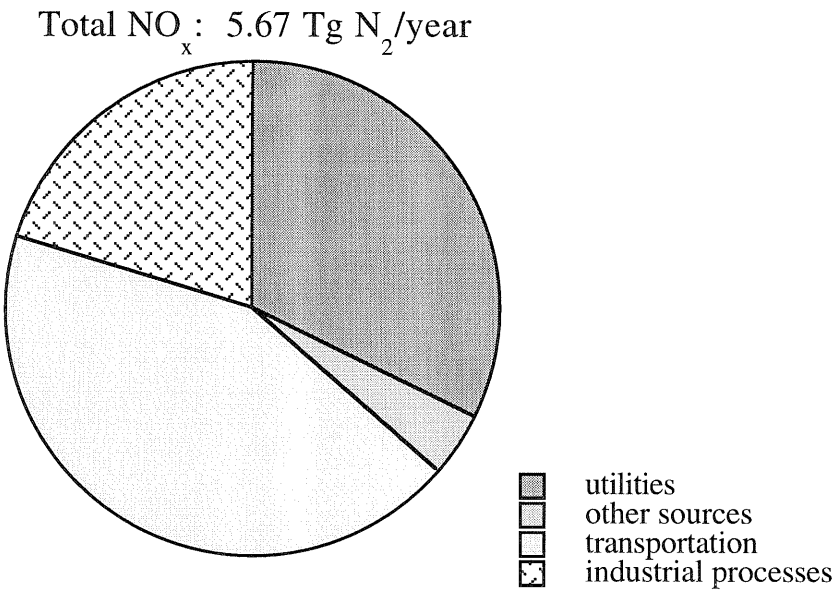

Figure 1.1. Emission and Sources of NO_X, 1985 (National Research Council, 1991).

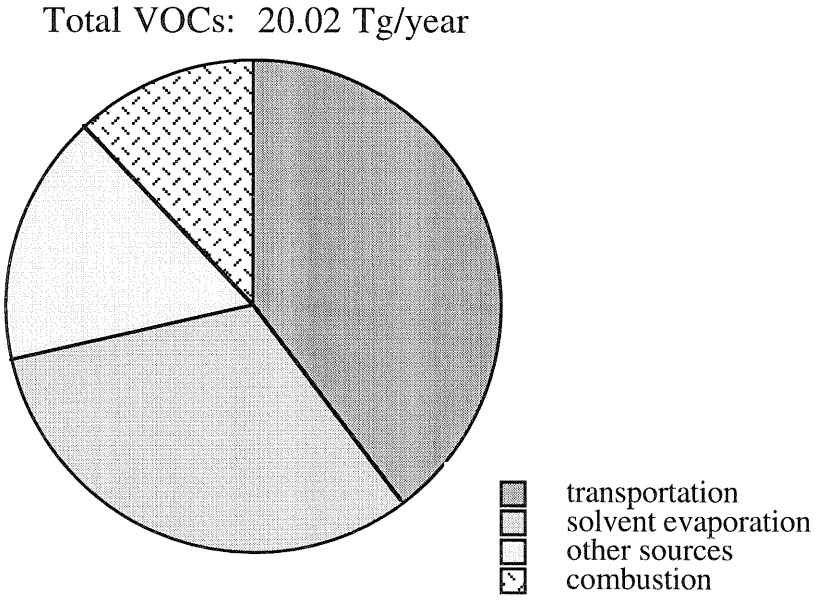

Figure 1.2. Emission and Sources of VOCs, 1985 (National Research Council, 1991).

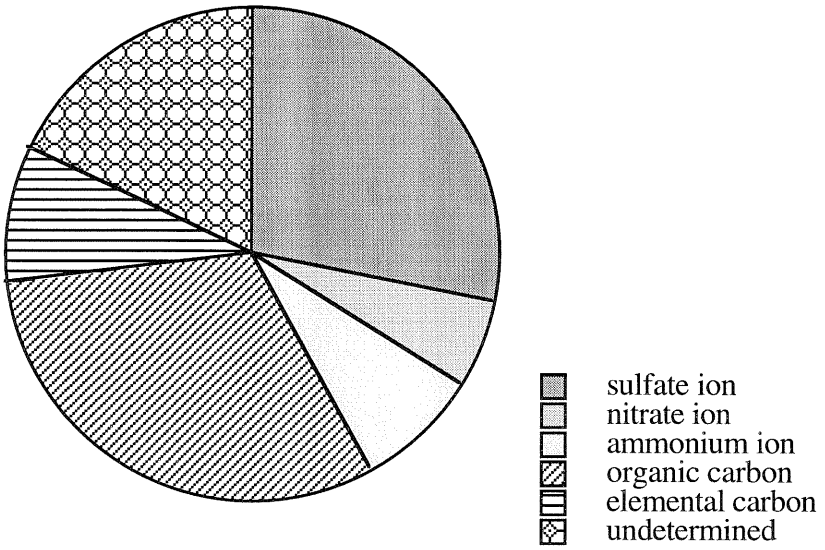

Figure 1.3. Average urban fine particle composition (Heintzenberg, 1989).

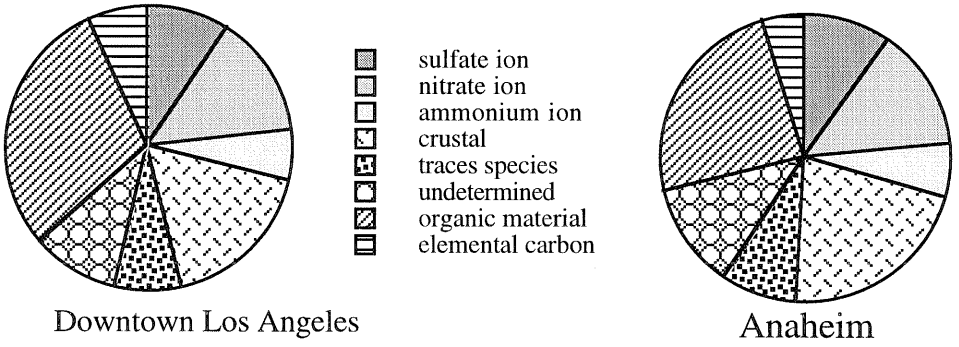

Figure 1.4. Annual average PM_{10} aerosol composition in 1986 (Solomon *et al.,* 1989).

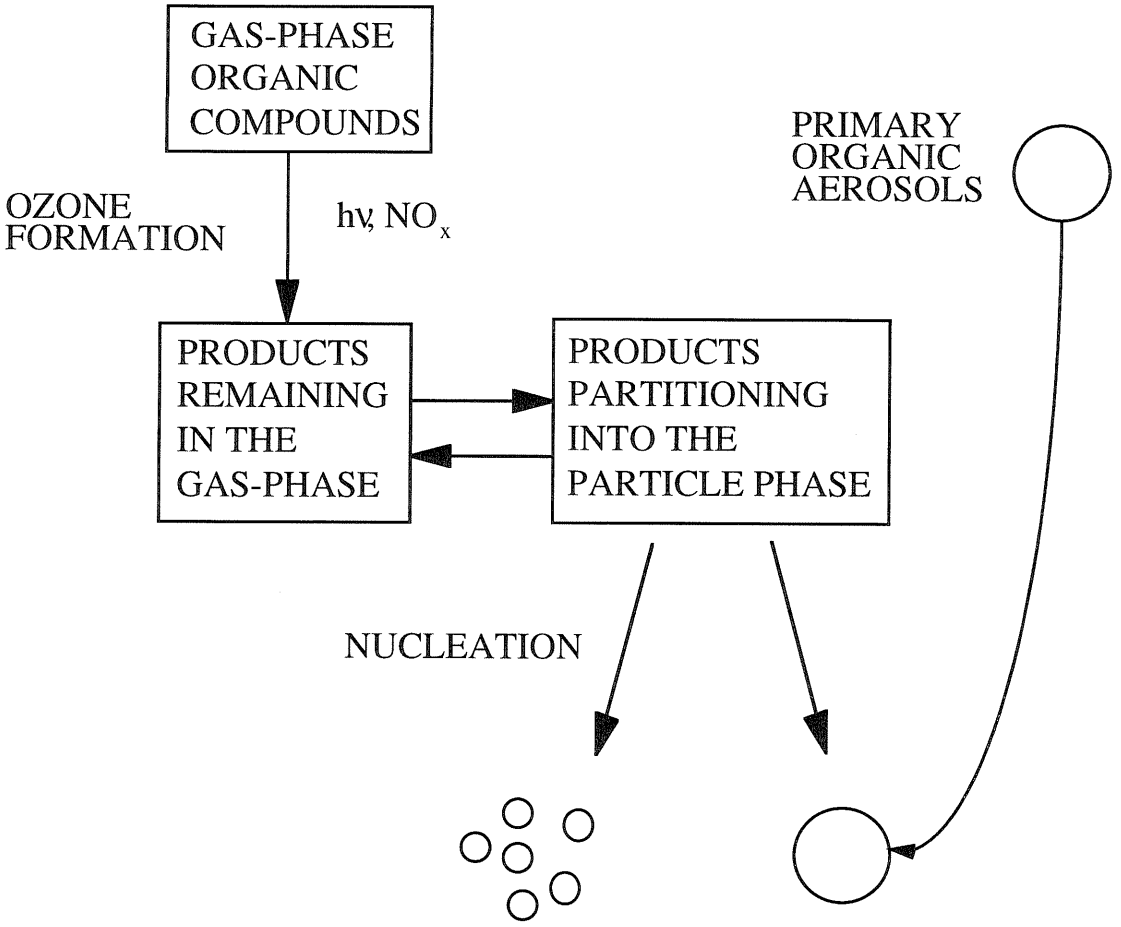

Figure 1.5. Gas-to-Particle Conversion.

Table 1.1. SCAQS Morning Composition of Nonmethane Organic Compounds.[a]

COMPOUND	% NMOC	COMPOUND	% NMOC
propane	7.888	2,3,4-trimethylpentane	0.381
toluene	7.876	3-methylheptane	0.377
isopentane	7.841	*n*-decane	0.353
n-butane	6.166	1-pentene	0.347
ethane	4.538	trans-2-pentene	0.324
ethene	4.202	butanal	0.296
n-pentane	3.709	1,3-butadiene	0.282
acetylene	3.007	isoprene	0.279
isobutane	2.820	*n*-propylbenzene	0.278
benzene	2.776	nonane	0.271
2-methylpentane	2.545	C_7 carbonyl	0.270
p-xylene	2.442	*cis*-2-pentene	0.263
m-xylene	2.442	4-methyloctane	0.209
acetone	2.359	3-methyloctane	0.209
o-xylene	1.805	*trans*-2-butene	0.185
3-methylpentane	1.789	C_5 carbonyl	0.184
n-hexane	1.750	*cis*-2-butene	0.181
methylcyclopentane	1.721	2,2,5-trimethylhexane	0.170
propylene	1.680	cycloheptane	0.110
1,2,4-trimethylbenzene	1.656	3-methyl-1-butene	0.098
2,2,4-trimethylpentane	1.414	2-methyl-2-pentene	0.093
ethylbenzene	1.292	3,3-dimethylpentane	0.083
acetaldehyde	1.226	2,5-dimethylheptane	0.067
3-methylhexane	1.167	2,2-dimethylbutane	0.037
methylcyclohexane	1.100	1-nonene	0.029
pentanal	1.088	3-methyl-trans-2-pentene	0.017
formaldehyde	1.042	1-octene	b
methylethylketone	1.035	2,2,3-trimethyl-1-butene	b
C_6 carbonyl	1.034	2,3-dimethylheptane	b
m-ethyltoluene	1.008	2,3-dimethylhexane	b
2-methylhexane	0.981	2,4-dimethylheptane	b
n-heptane	0.958	2,4-dimethylhexane	b
1-butene	0.743	2,5-dimethylhexane	b
2,3-dimethylbutane	0.686	2-methylpropene	b
2,3-dimethylpentane	0.662	4-methyl-1-pentene	b
p-ethyltoluene	0.522	α-pinene	b
propanal	0.505	*cis*-2-octene	b
cyclohexane	0.493	*cis*-3-methyl-2-pentene	b
2,4-dimethylpentane	0.451	*cis*-4-methyl-2-pentene	b
o-ethyltoluene	0.448	cyclohexene	b
cyclopentane	0.433	ethylcyclohexane	b
2-methyl-1-butene	0.423	3-methylcyclohexene	b
2-methylheptane	0.409	*trans*-4-methyl-2-pentene	b
n-octane	0.389	trichloroethene	b

[a]Adapted from Lurmann and Main (1992)

[b]Detected, but below the limit to assign a percentage

Table 1.2. Studies on Secondary Aerosol Formation.

COMPOUNDS	FAC:NO_x[a] %	AEROSOL SPECIES IDENTIFIED	RESEARCHER	YEAR
Alkanes				
n-heptane	<0.06		McMurry, Grosjean	1985
n-octane	<0.001		Wang	1992
2,6-dimethylheptane	0.65		O'Brien	1975
cyclohexane	<0.017		McMurry, Grosjean	1985
methylcyclohexane	9.2		Wang	1992
Aromatics				
benzene	0		multiple (incl. Izumi)	1990
toluene	1.0-3.0		Grosjean	1978
	0.6-1.4		Leone	1985
	2.1		Stern	1987
	0.5-1.7		Gery	1985
	2.3		Izumi	1990
	6.4		Wang	1992
m-, *o*-, *p*-ethyltoluene	1.9, 1.4, 0.6		Izumi	1990
o-xylene	6.2		O'Brien	1975
m-xylene	2.9		Stern	1987
m-, *o*-, *p*-xylene	2.5-3.1, 2.1, 0.73		Izumi	1990
ethylbenzene	0.6		Stern	1987
	0.78		O'Brien	1975
	2		Izumi	1990
n-propylbenzene	0.2		Izumi	1990
isopropylbenzene	1		Izumi	1990
1,2,3-trimethylbenzene	1.4		Izumi	1990
1,2,4-trimethylbenzene	0.6		Izumi	1990
1,3,5-trimethylbenzene	1.2		Izumi	1990
	2.1		Stern	1987
	0.69-1.92		O'Brien	1975
Phenols				
o-cresol	0.5-14.0 / 0[b]	2-hydroxy-3-nitrotoluene 2-hydroxy-5-nitrotoluene 2-hydroxy-3,5-dinitrotoluene	McMurry, Grosjean	1985
4-hydroxy-2-nitrotoluene	8.6	3,5-dinitro-4-hydroxytoluene	McMurry, Grosjean	1985
Esters				
methoxybenzene	0.8		Izumi	1990
Olefins				
1-hexene	0.34 / 0.24[b]		McMurry, Grosjean	1985
1-heptene	0.85		O'Brien	1975
	18[b]	hexanoic acid	Grosjean	1984
1-octene	4.2	5-propyl furanone heptanoic acid	Wang	1992
cyclopentene	1.0-5.0[b]	succinic acid glutaraldehyde	Hatakeyama	1987

		5-oxo-pentanoic acid glutaric acid		
cyclohexene	18.3		Izumi	1988
	13[b]	adipaldehyde 6-oxo-hexanoic acid adipic acid gluataraldehyde 5-oxo-pentanoic acid glutaric acid	Hatakeyama	1987
cycloheptene	4.0-10.0[b]	glutaric acid adipaldehyde 6-oxo-hexanoic acid adipic acid pimelaldehyde 7-oxo-heptanoic acid pimelic acid	Hatakeyama	1987
isoprene	0		Paulson	1991
indene	+		O'Brien	1975
1,5-hexadiene	20.3		O'Brien	1975
1,6-heptadiene	69		O'Brien	1975
2-methyl-1,5-hexadiene	47.6		O'Brien	1975
1,7-octadiene	68		O'Brien	1975
	10.3		Grosjean, Friedlander	1979
2,6-octadiene	0.9		O'Brien	1975
Terpenes				
α-pinene	55		O'Brien	1975
	38-55		Hooker	1985
	18.3[b]	pinonaldehyde nor-pinonaldehyde pinonic acid nor-pinonic acid	Hatakeyama	1989
β-pinene	8	nopinone pinocamphone	Pandis	1990
	13.8[b]	nopinone	Hatakeyama	1989
limonene	>50		Schuetzle	1978
Other				
styrene	0.5		Izumi	1990
α-, β-methylstyrene	1.3-7.6, 1.0		Izumi	1990

[a] Fractional aerosol coefficient (FAC) is the percentage of the mass concentration of aerosol formed to the initial mass concentration of the hydrocarbon precursor.

$$FAC = 100\ \frac{aerosol\ from\ reactive\ organic\ gases\ \mu g\ m^{-3}}{initial\ reactive\ organic\ gases\ \mu g\ m^{-3}}$$

[b] FAC determined from the photooxidation of the hydrocarbon with only ozone, rather than in the presence of nitrogen oxides.

CHAPTER 2

Secondary Organic Aerosol Formation from the Photooxidation of Aromatic Hydrocarbons. I. Aerosol Yields

Abstract

Outdoor smog chamber experiments have been performed to determine the secondary organic aerosol (SOA) formation potential of various C_7, C_8, and C_9 aromatics in sunlight-irradiated hydrocarbon-NO_x mixtures. Measured aerosol yields from toluene, *m*-xylene, *p*-xylene, ethylbenzene, *m*-ethyltoluene, *p*-ethyltoluene, and 1,2,4-trimethylbenzene were found to correlate with organic mass concentration according to semi-volatile gas/particle partitioning theory. Aerosol yields of the C_9 aromatics were greater than those of the C_8 aromatics, with *m*-ethyltoluene resulting in the greatest yields. Toluene and ethylbenzene demonstrated some aerosol-forming potential, but the other aromatics produced significantly more SOA.

Introduction

Urban aerosol frequently contains a substantial fraction of elemental and organic carbon (Solomon *et al.*, 1986; Turpin and Huntzicker, 1991; Rogge *et al.*, 1991, 1993abcd). The organic carbon component arises from both direct emissions and photooxidation of gas-phase organics with subsequent gas-to-particle conversion of oxidation products. Evidence of secondary organic aerosol is suggested when the ambient organic to elemental carbon (OC/EC) ratio is higher than that at emission sources. During the 1987 Southern California Air Quality Study (SCAQS), Turpin and Huntzicker (1991) found that coincidence of high ozone levels with a lack of correlation between OC and EC profiles suggested significant secondary organic aerosol formation. In the pollution episode of 25-31 August 1987, Turpin and Huntzicker (1991) estimated the secondary organic aerosol contribution to be approximately 70% by mass of the total organic aerosol.

Aerosol yield resulting from the oxidation of a gas-phase organic has been defined as the ratio of secondary aerosol produced (in terms of volume or mass concentration) to the amount of hydrocarbon reacted (Stern *et al.*, 1987; Wang *et al.*, 1992). Historically, smog chamber studies have provided yield data by allowing measurement of secondary organic aerosol (SOA) produced from the photooxidation of a hydrocarbon in the presence of nitrogen oxides in a controlled environment. Aromatic hydrocarbons have been extensively investigated because they are known to form secondary photooxidation products leading to aerosol formation, and all significantly contributed to the total gas-phase organic compound concentration in Los Angeles, as measured during SCAQS (Lurmann and Main, 1992). Table 2.1 summarizes previously reported aerosol yields of aromatic compounds (Izumi and Fukuyama, 1990; Grosjean *et al.*, 1978; Leone *et al.*, 1985; Stern *et al.*, 1987; Gery *et al.*, 1985; O'Brien *et al.*, 1975; Grosjean, 1985). The first column lists the aerosol yields as reported in the literature and the second column lists recalculated fractional aerosol coefficients (FAC), according to the procedure outlined in Grosjean and Seinfeld (1989).

One of the notable features of the data in Table 2.1 is the wide range of reported yields for almost all aromatic precursors.

Viewing secondary organic aerosol species as semi-volatile compounds and utilizing Pankow's (1994ab) gas/particle partitioning absorption model, Odum *et al.* (1996) demonstrated that secondary organic aerosol yield is not a constant for an individual hydrocarbon, but rather is a function of the organic aerosol mass concentration present. The reason for this dependence is that the organic aerosol mass serves as the particulate-phase medium into which the gas-phase species are absorbed, and therefore the amount of organic aerosol mass directly affects the gas/particle partitioning.

We report here the results of a series of smog chamber experiments performed to measure the aerosol yields of aromatic hydrocarbons during photooxidation in the presence of NO_X: toluene, *m*-xylene, *p*-xylene, ethylbenzene, *m*-ethyltoluene, *p*-ethyltoluene, and 1,2,4-trimethylbenzene. Gas/particle partitioning theory was applied to the above smog chamber experiments and found to adequately describe the results, providing further evidence for the applicability of semi-volatile gas/particle absorption theory to secondary organic aerosol formation.

Experimental

Outdoor Smog Chamber System

The experiments were performed in a flexible, outdoor smog chamber, similar to that originally described by Pandis *et al.* (1991) and Wang *et al.* (1992). The chamber was constructed of 2 mil thick Teflon film. The chamber was operated such that two experiments could be conducted simultaneously. This dual-chamber mode was achieved by placing a PVC pipe across the chamber, effectively dividing it into two smaller chambers each with a volume of approximately 19 m^3. The smog chamber was supported 0.6 m above the rooftop, allowing for circulation of air beneath the chamber and thereby

reducing warming of the chamber. The area underneath the chamber was painted black to lessen any reflection of radiation. The chamber contents were well-mixed due to the wind causing undulations in the flexible chamber walls.

The night before an experiment, the chamber was covered with a black tarpaulin and inflated with purified air. Laboratory compressed air was passed through three packed beds. The first bed contained activated charcoal to remove hydrocarbons; the second contained Purafil for the removal of NO_X from the air stream; and the last bed contained in equal parts silica gel and 13X molecular sieves to remove water and carbon dioxide. After passing through the three beds, the air was passed through a total particle filter and was then humidified to at least 15% relative humidity. The following morning the reactants were injected into the chamber. A known volume of the liquid hydrocarbon was injected into a glass bulb. The bulb was gently heated as air flowed through it to the chamber, evaporating the hydrocarbon into the air stream. Nitric oxide, nitrogen dioxide, and propene were injected into the chamber using cylinders (Matheson Gas Products Inc.) containing several hundred ppm of the gas in ultra-pure nitrogen. Propene was injected into the chamber in order to generate hydroxyl radicals from the chemistry of ozone addition to the propene molecule. Seed particles were added last to the chamber to minimize particle losses to the walls. The initial aerosol was generated by atomizing a dilute solution of ammonium sulfate. The aqueous ammonium sulfate droplets were dried and then passed through a ^{85}Kr decharger prior to entering the chamber. After allowing the contents of the chamber sufficient time to mix and the initial gas-phase and aerosol phase measurements to stabilize, the cover was removed, exposing the chamber to sunlight and initiating the photochemical reactions.

The gas-phase instruments and the data acquisition systems for both gas and particle measurements were indoors in a laboratory next to the chamber. The aerosol instruments were placed in a cart immediately adjacent to the Teflon chamber in order to minimize the

length of the aerosol sampling lines. The temperature inside the cart was maintained between 21 and 25 °C. The gas-phase sampling lines were Teflon, while the aerosol lines were copper to minimize depositional losses. The gas-phase, on-line measurements included NO, NO_X, O_3 and the hydrocarbons of interest. Ozone was measured with a Dasibi model 1008-PC analyzer (Glendale, CA), which was calibrated by the South Coast Air Quality Management District (Diamond Bar, CA). NO and NO_X were monitored with a Thermo Environmental Instruments Inc. (Franklin, MA) Model 42 chemiluminescence NO-NO_2-NO_X analyzer. The NO_X analyzer was calibrated in-house using certified (±2% tolerance) cylinders of NO in oxygen-free nitrogen (Scott-Marrin Inc., Riverside, CA). Hydrocarbons were monitored by a Hewlett Packard 5890 gas chromatograph equipped with flame ionization detector (FID) and a DB-5 (30 m, 0.25 mm ID, 0.25 μm phase thickness) column (J&W Scientific). Gas-phase samples were injected into the GC using a six-port valve (VICI, Valco Instruments Co. Inc., Houston, TX) to sample automatically every 15 minutes throughout the run. The gas chromatograph was calibrated after every experiment using certified (±2% tolerance) cylinders (Scott-Marrin Inc., Riverside, CA) containing each hydrocarbon in nitrogen. The standard error in the O_3 measurements was ±2 ppb, and the resulting error in peak ozone measurements was significantly less than 1%. Rigorous statistical analyses of the NO_X and hydrocarbon measurements were performed. The probable error in the NO, NO_2, and NO_X monitor values were typically ±7, ±18, and ±11 ppb respectively. This error amounted to less than ±2.4%, ±13%, and ±2.4% of the initial measured concentrations of NO, NO_2 and NO_X respectively. The probable errors in the hydrocarbon measurements ranged from ±5 ppb to ±103 ppb, which is ±2% to ±30% of the initial hydrocarbon concentrations. The error in the aerosol yields can be attributed to the error in the gas chromatograph measurements.

The aerosol instrumentation included two differential mobility analyzers (DMA, TSI Model 3071) and two condensation nuclei counters (CNC, TSI model 3760). The DMAs

and CNCs were operated as scanning electrical mobility spectrometers (SEMS) (Wang and Flagan, 1990) and generated particle size distributions every minute with a size range of about 10 nm to 200 nm. The DMAs were calibrated with polystyrene latex particles (PSL) of known size, 0.198 μm.

The initial conditions for the smog chamber experiments are listed in Table 2.2. The initial hydrocarbon mixing ratios ranged from 200 to 900 ppb, and the initial propene mixing ratios ranged from 100 to 340 ppb. Propene was added to the smog chamber to enhance photochemical reactivity (Wang *et al.*, 1992). It is important to note that although the initial hydrocarbon concentrations are one to two orders of magnitude greater than ambient levels, the hydroxyl radical chemistry of the aromatic is expected to be the same as under ambient conditions, and hence, the results are valid for atmospheric conditions. Initial hydrocarbon-NO_X ratios ranged from 3 to 14 ppbC/ppb, similar to those measured during SCAQS (Lurmann and Main, 1992). Ammonium sulfate seed aerosol was used to encourage condensation of the secondary gas-phase products. Initial seed particles were introduced at a number concentration of approximately 2000 cm^{-3}. The initial particle number concentration was lower than that in the ambient in order to allow observation of growth of the seed aerosol, as a measure of secondary aerosol formation. The initial particle size distribution included particles from 10 nm in diameter to about 200 nm, with the distribution generally centered at 65 nm.

Aerosol Yield

Aerosol yield from the photooxidation of a hydrocarbon can be expressed in several ways. (See Table 2.1.) A convenient definition of yield is the ratio of the volume concentration of aerosol formed to the amount of hydrocarbon reacted. The aerosol yield Y is a function of time during photooxidation. Expressed in units $\mu m^3\ cm^{-3}\ ppm^{-1}$, $Y(t)$ is then:

$$Y(t) = \frac{V(t) - V_O}{[HC]_O - [HC(t)]} \tag{1}$$

where $[HC]$ is the hydrocarbon concentration expressed in units of ppm, and V_O is the initial volume of seed aerosol expressed in units of $\mu m^3\ cm^{-3}$. Given an aerosol density, the yield can also be expressed on a mass basis. Stern *et al.* (1987) assumed that the density of secondary organic aerosol was 1.0 $g\ cm^{-3}$, and upon converting the hydrocarbon concentration from units of ppm to units of $\mu g\ m^{-3}$, the aerosol yield is expressed on a mass basis. Table 2.3 lists the densities and molecular weights of various species identified in secondary organic aerosol from smog chamber studies of aromatic photooxidation (Forstner *et al.*, 1996). A density of 1 $g\ cm^{-3}$ is seen to be a reasonable approximation for the SOA products. Izumi and Fukuyama (1990) expressed aerosol yield on a carbon basis. They measured the aerosol density to be $0.49 \pm 0.02\ gC\ cm^{-3}$, and to be largely independent of the particular hydrocarbon. The fraction of hydrocarbon reacted was also expressed on a carbon mass basis and the aerosol carbon yield (Y_C) is:

$$Y_C(t) = \frac{0.49\ (\ V(t)\ -\ V_O)}{f_C\ (\ [HC]_O - [HC(t)]\ )} \tag{2}$$

where f_C is a constant to convert hydrocarbon concentration in units of ppm to carbon mass concentration. By assuming an average molecular weight of the species in the particle phase to be 150 $g\ mol^{-1}$, Izumi and Fukuyama's aerosol density can be placed on a mass basis and is approximately 0.9 g cm-^{3}. Although Stern *et al.* (1987), Wang *et al.* (1992), and Izumi and Fukuyama (1990) used similar approaches to determine aerosol yield for several aromatics, they did not arrive at consistent yields, as shown in Table 2.1. It

appears that the above definitions of aerosol yield do not fully account for the complex processes involved in secondary organic aerosol formation.

Odum *et al.* (1996) departed from the above definitions of aerosol yield as a constant parameter, and considered secondary aerosol formation in the framework of Pankow's (1994ab) gas/particle partitioning absorption model. In this model the production of secondary organic aerosol is controlled by an equilibrium partitioning of the semi-volatile compound between the gas-phase and the organic matter phase. Then the partitioning of gas-phase organics into the particle phase may occur even when the gas-phase partial pressure of a compound is below its saturation vapor pressure. Gas/particle partitioning is represented by a partitioning constant for compound *i*:

$$K_{p,i} = \frac{F_{i,om}}{A_i \, TSP} \tag{3}$$

where *TSP* is the concentration of total suspended particulate matter (μg m^{-3}), and $F_{i,om}$, and A_i are the particulate-associated (ng m^{-3}) and gaseous concentrations (ng m^{-3}) of compound i , respectively. The partitioning constant can then be defined as:

$$K^i_{om} = \frac{F_{i,om}}{A_i \, M_O} \tag{4}$$

where K^i_{om} is a partitioning coefficient (m^3 μg^{-1}), M_O is the organic mass concentration (μg m^{-3}), and $F_{i,om}$ is the concentration of compound i in the organic matter phase (ng m^{-3}). By assuming that the total concentration of compound i in the gas-phase and in the particle phase is proportional (α_i) to the amount of parent hydrocarbon that has reacted, Odum *et al.* (1996) developed an expression for the aerosol yield using equations (1) and (4),

$$Y(t) = M_O(t) \sum_i \frac{\alpha_i K^i_{om}}{1 + K^i_{om} M_O(t)} \tag{5}$$

where $M_O(t)$ denotes the total organic aerosol mass concentration at time t, α_i is the stoichiometric coefficient relating the concentration of hydrocarbon reacted to the total

concentration of product formed, and K^i_{om} is the partitioning coefficient. This expression demonstrates that aerosol yield is a function of the organic mass concentration present in the smog chamber. Odum *et al.* (1996) calculated the organic aerosol mass concentration from the aerosol volume concentrations measured during their experiments, assuming a density of 1.0 g cm^{-3}, and then fitted parameters (α_1, α_2, K^1_{om}, K^2_{om}) to the data. A two-product model was found to be necessary to fit the behavior of the system. A one-product model is insufficient to represent the data, and a three-product model provides an unnecessary amount of freedom.

In this study, the aerosol yield was calculated according to equation (1). Particle size distributions were measured with a Scanning Electrical Mobility Spectrometer (Wang and Flagan, 1990). The data were corrected for wall losses (see Appendix at end of chapter), then integrated to determine the secondary aerosol volume concentration, $V(t)$, and converted to a mass basis assuming an aerosol density of 1.0 g cm^{-3}. All data to be presented have an uncertainty associated with each measured aerosol yield. This error arises primarily from uncertainty in the hydrocarbon measurements, which themselves result from the inconsistency of the gas chromatograph response. The measured aerosol volume is virtually entirely secondary organic product, that is $V(t) >> V_o$. Since the relative humidity of the smog chamber was typically 30% or less at temperatures around 303K, water is not likely to be present in the aerosol phase, and the initial volume of seed aerosol is on the order of 0.01% to 1% of the final aerosol volume.

Measured Aerosol Yields

Fifty-four individual outdoor smog chamber experiments were run over 27 days in 1994 (Table 2.2). Gas/particle partitioning theory suggests that $Y(t)$ should depend on $M_O(t)$ according to equation (5). Thus, yield data will be presented as $Y(t)$ versus $M_o(t)$. In the ensuing figures, not all experiments are shown in order for clarity in the region near the origin.

SOA yields from individual experiments for *p*-ethyltoluene are shown in Figure 2.1. The solid line in Figure 2.1, and those in later figures, was generated from equation (5) using a two-product model, where α_1, α_2, K^1_{om}, *and* K^2_{om} were fitted to the data. The best fit parameters for each of the aromatics are listed in Table 2.4. Figure 2.2 shows yield versus organic mass concentration for individual 1,2,4-trimethylbenzene experiments along with the line generated from equation (5) using the values for α_1, α_2, K^1_{om}, and K^2_{om} of Odum *et al.* (1996). Data from *p*-xylene experiments are shown in Figure 2.3. The discrepancy between the 21 August experiment and the 23 August can be explained by considering the effect of temperature. During the course of an experiment, the formation of SOA typically occurs in the afternoon. Afternoon temperatures were between 34 to 38 °C on 23 August and between 36 to 40 °C on 21 August. At higher temperatures, the vapor pressures of the secondary organics increase; consequently, gas/particle partitioning favors the gas phase, and SOA yields decrease. Hence the yields for the 21 August experiment are lower. Aerosol yields for *m*-ethyltoluene experiments are shown in Figure 2.4. Again, a single curve of yield against organic mass concentration results.

Ethylbenzene and toluene SOA yields are shown in Figure 2.5. As compared to *m*-xylene, for example, insufficient secondary organic aerosol formed from toluene and ethylbenzene to generate enough data to fit parameters to yield curves. The values for α_1, α_2, K^1_{om}, and K^2_{om} for toluene and ethylbenzene given in Table 2.4 must consequently be viewed as provisional. Individual *m*-xylene experiments are shown in Figure 2.6, along

with the fit of Odum *et al.* (1996). The data conform to equation (5) and closely match Odum *et al.*'s (1996) fit with the exception of the experiment of 4 September. Whereas a possible reason for this discrepancy could be the effect of temperature, the experiments on 19 and 21 August and 4 September were conducted at similar afternoon temperatures. A different reason could be rooted in the assumption that the amount of SOA product is proportional to the amount of aromatic reacted. Odum *et al.* (1996) noted that the products must react at similar rates as the parent aromatic in order for this assumption to be correct. It is possible that on 4 September this assumption does not hold, and that the products are not reacting as quickly as the parent aromatic, allowing for the accumulation of product and hence greater yields. The difference in peak ozone concentrations (see Table 2.2) between the 4 September and the August *m*-xylene experiments indicates a difference in reactivities of the smog chamber on those days, and suggests that the above explanation is plausible. The difference in aerosol yield for the 21 and 23 August *p*-xylene experiments may also be attributed to the secondary products not reacting at a rate similar to that of *p*-xylene itself.

Figure 2.7 compares the best fit parameters of equation (5) for all aromatics. The inset in Figure 2.7 is the region from 0 to 5 $\mu g\ m^{-3}$ of SOA with only toluene, ethylbenzene, *p*-xylene, *m*-ethyltoluene, and *p*-ethyltoluene shown. The greatest yields were attained with *m*-ethyltoluene. Overall, the C_9 aromatics have greater yields than the C_8 aromatics. Because the first generation photooxidation products of C_9 aromatics will have in general one more carbon than the C_8 products, these organics should have lower vapor pressures thereby partitioning more into the particle-phase. Hence, the greatest yields were attained with *m*-ethyltoluene, then *p*-ethyltoluene, and then 1,2,4-trimethylbenzene. The hydroxyl radical rate constant for 1,2,4-trimethylbenzene is $32.5 \pm 1.1 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, 17.0 ± 3.4 for *m*-ethyltoluene, and 11.3 ± 2.3 for *p*-ethyltoluene. It might be anticipated that 1,2,4-trimethylbenzene would exhibit the highest yields since it is the most reactive of the C_9 aromatics. If, however, the photooxidation products of 1,2,4-trimethylbenzene are

themselves highly reactive with hydroxyl radicals as compared to the photooxidation products of *m*- or *p*-ethyltoluene, then there would be less opportunity, before subsequent reaction for the 1,2,4-trimethylbenzene products, to accumulate and partition into the particle phase. Also, the 1,2,4-trimethylbenzene products may be more volatile than the photooxidation products of *m*- or *p*-ethyltoluene, and hence will partition less into the particle phase, thereby decreasing aerosol yield. Although the toluene fit falls on the 1,2,4-trimethylbenzene fit, and the ethylbenzene fit falls on the *m*-xylene fit, based on the available data, the only conclusion that can be drawn is that toluene and ethylbenzene exhibit smaller aerosol-forming potential compared to the other aromatics studied. Initially the SOA yields of *m*-xylene exceed those of *p*-xylene, until the organic mass concentration reaches approximately 30 $\mu g\ m^{-3}$, and then *p*-xylene yields are greater. No particular mechanistic conclusion can be drawn from this behavior at this time. For the other aromatics, when the particle size distributions grew beyond the range of the SEMS, the data are limited to a smaller range of organic mass concentrations, and consequently we cannot determine if other yield curves cross.

Conclusions

A series of outdoor smog chamber experiments were performed during the summer of 1994 to measure the secondary organic aerosol yields of toluene, ethylbenzene, *m*-xylene, *p*-xylene, *m*-ethyltoluene, *p*-ethyltoluene and 1,2,4-trimethylbenzene. For all aromatics, the aerosol yield was found to correlate with organic mass concentration according to semi-volatile gas/particle partitioning theory. The greatest yields were attained, in order, from *m*-ethyltoluene, *p*-ethyltoluene, 1,2,4-trimethylbenzene, and *m*-xylene and *p*-xylene. Insufficient data for toluene and ethylbenzene were available to draw definitive conclusions.

Appendix: Wall Loss Measurements

A theory of wall deposition of particles in vessels was developed by Crump and Seinfeld (1981), who developed a general theory for the rate of aerosol deposition due to turbulent diffusion, Brownian diffusion, and gravitational sedimentation in a turbulently mixed vessel. McMurry and Rader (1985) extended this theory to include electrostatic effects, typically associated with Teflon smog chambers. These analyses resulted in a comprehensive model of particle loss in smog chambers, accounting for particle transport by convection, Brownian diffusion, gravitational sedimentation, and electrostatic drift. Charged particles are lost more quickly to smog chamber walls than neutral particles, and consequently, the wall deposition rates of particles are time dependent because charged particles are removed preferentially at first. McMurry and Rader (1985) applied their model to calculate size-dependent wall deposition rates in a Teflon film smog chamber, and found that their model was in good agreement with the experimental wall loss data.

Rather than attempting to incorporate McMurry and Rader's model directly, in the present study an empirical expression was found to correlate well with the significantly more complex model of McMurry and Rader. The wall loss expression was determined from three experiments which were performed to measure the loss rates of particles in the Caltech outdoor smog chamber. Ammonium sulfate particles ranging in diameter from 15 nm to 200 nm (*i.e.,* the seed aerosol in the experiments) were injected into the bag at concentrations similar to those used in the experiments. Using the SEMS instruments discussed above, the particle size distributions were measured over a period of five hours. The particles were separated into ten size bins, with bin 1 having a nominal diameter of 13.5 nm, bin 2 of 17.8 nm, bin 3 of 23.5 nm, bin 4 of 31.0 nm, bin 5 of 41.0 nm, bin 6 of 56.0 nm, bin 7 of 75.0 nm, bin 8 of 104 nm, bin 9 of 143 nm, and bin 10 of 187 nm. The SEMS inverted data for each size bin were then averaged over 10 min intervals. Figure 2.8 shows the deposition rate of particles for one experiment expressed as the fraction of the

initial particle concentration as a function of time. From these plots, a deposition rate (k, min^{-1}) was determined for each size bin. Similar rates were found for the other experiments. Figure 2.9 shows the deposition rate as a function of particle size. Points for the individual experiments are shown as well as an averaged data set. An expression was fitted to the averaged data with the form:

$$k = 10^{[3.54375 + 13.4646 \log D_p + 9.16105 (\log D_p)^2 + 1.8378 (\log D_p)^3]} \quad (6)$$

The data in Figure 2.9 closely resemble the results of McMurry and Rader (1985). The above expression was then used to correct the SEMS inverted data for particle losses to the chamber walls after accounting for multiple-charging effects. The deposition rate k was used to calculate the number of particles lost in a period of time. This loss was then added to the measurements made at that time.

Acknowledgments

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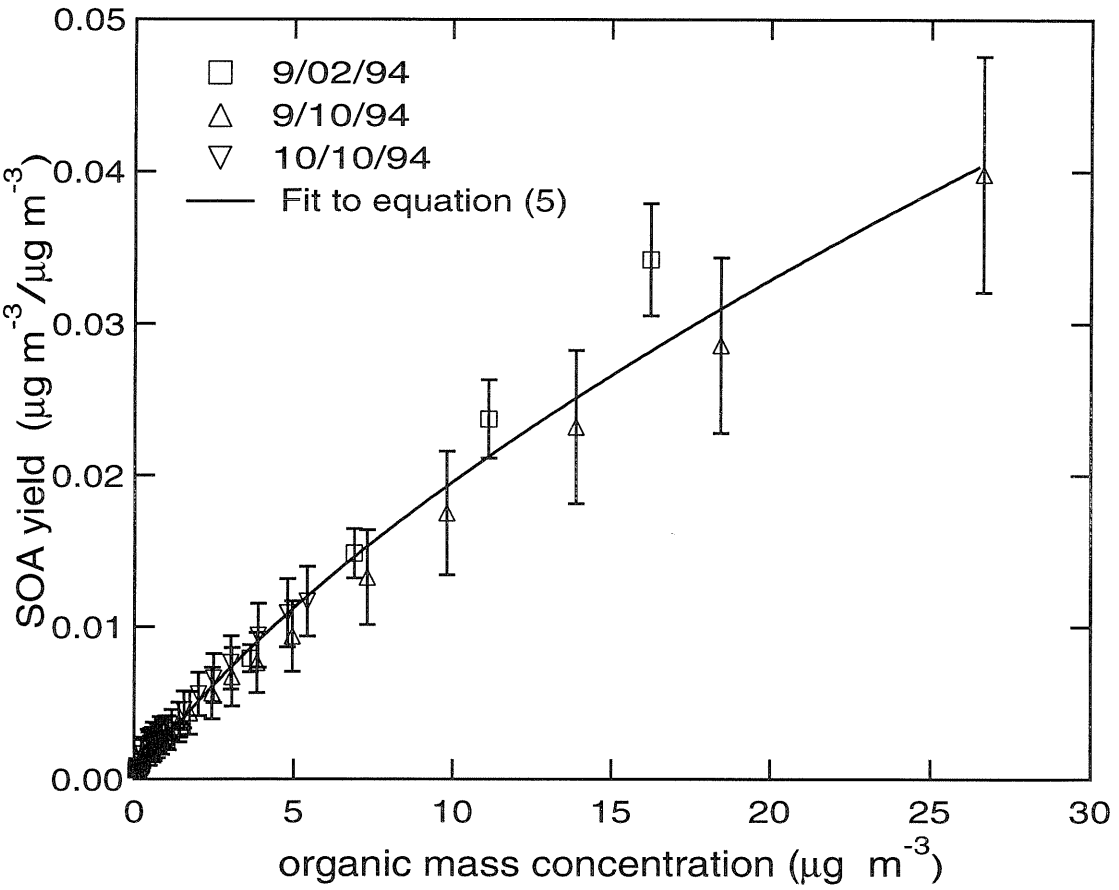

Figure 2.1. Time dependent SOA yields of individual *p*-ethyltoluene experiments as a function of organic mass concentration ($M_O(t)$). Equation (5) was fitted to the experimental data using a two-product model. Dates of experiments indicated (see Table 2.2).

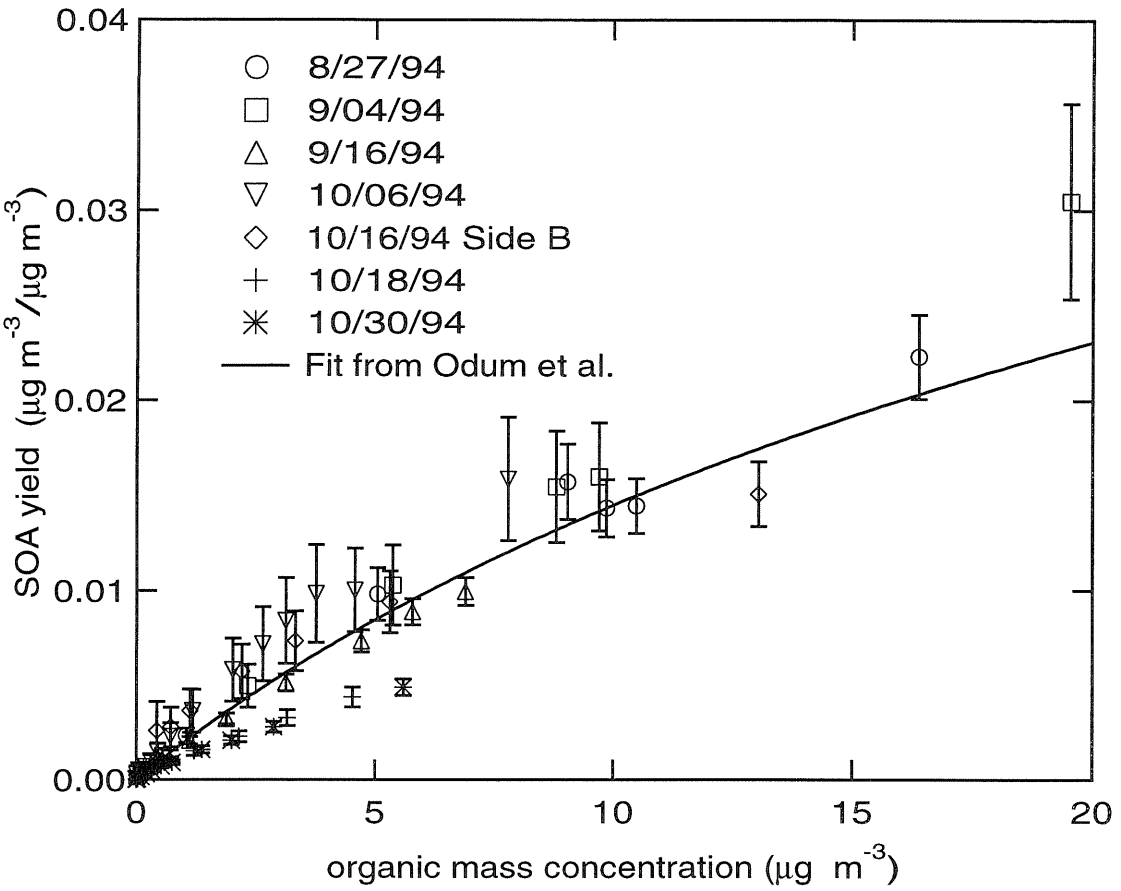

Figure 2.2. Time dependent SOA yields as a function of $M_O(t)$ for 1,2,4-trimethylbenzene. The fit from Odum *et al.* (1996) is included. Dates of experiments indicated (see Table 2.2).

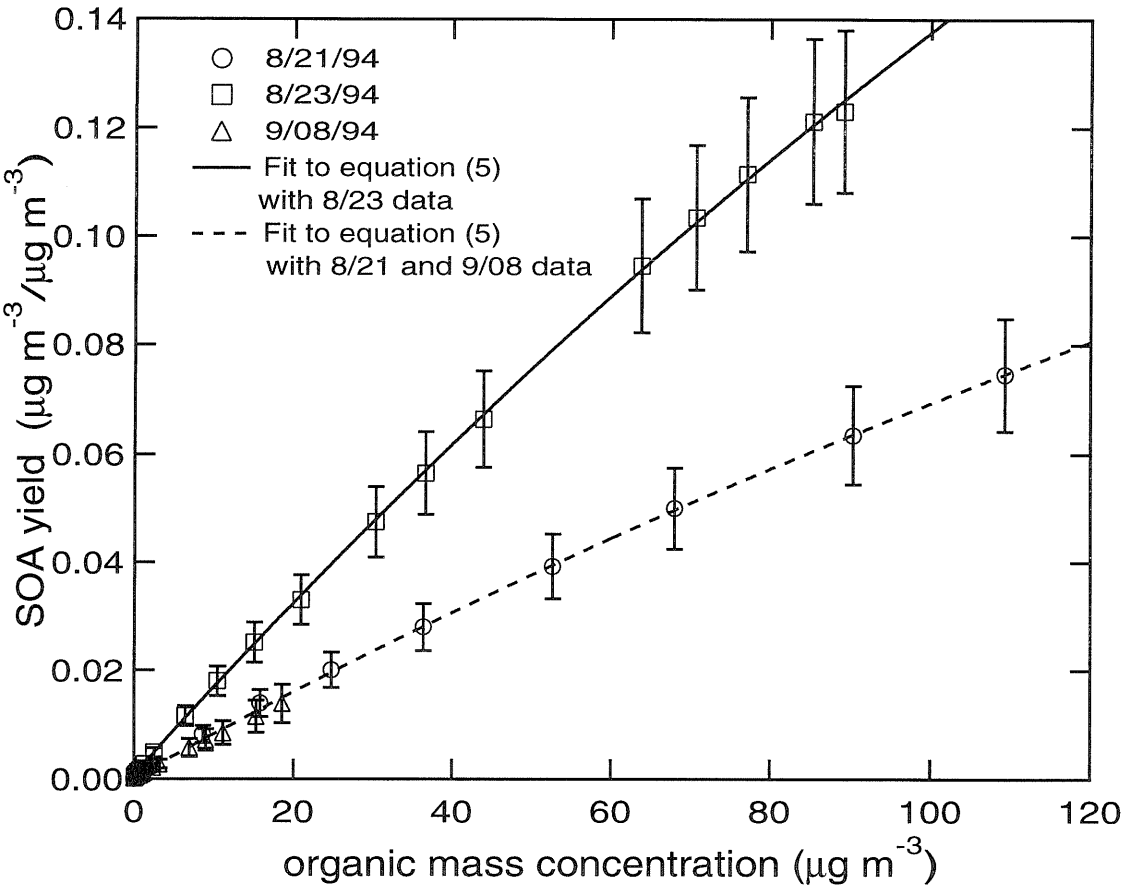

Figure 2.3. Time dependent SOA yields as a function of $M_O(t)$ for *p*-xylene. Equation (5) was fitted to the experimental data for 21 August and 23 August using a two-product model. Dates of experiments indicated (see Table 2.2).

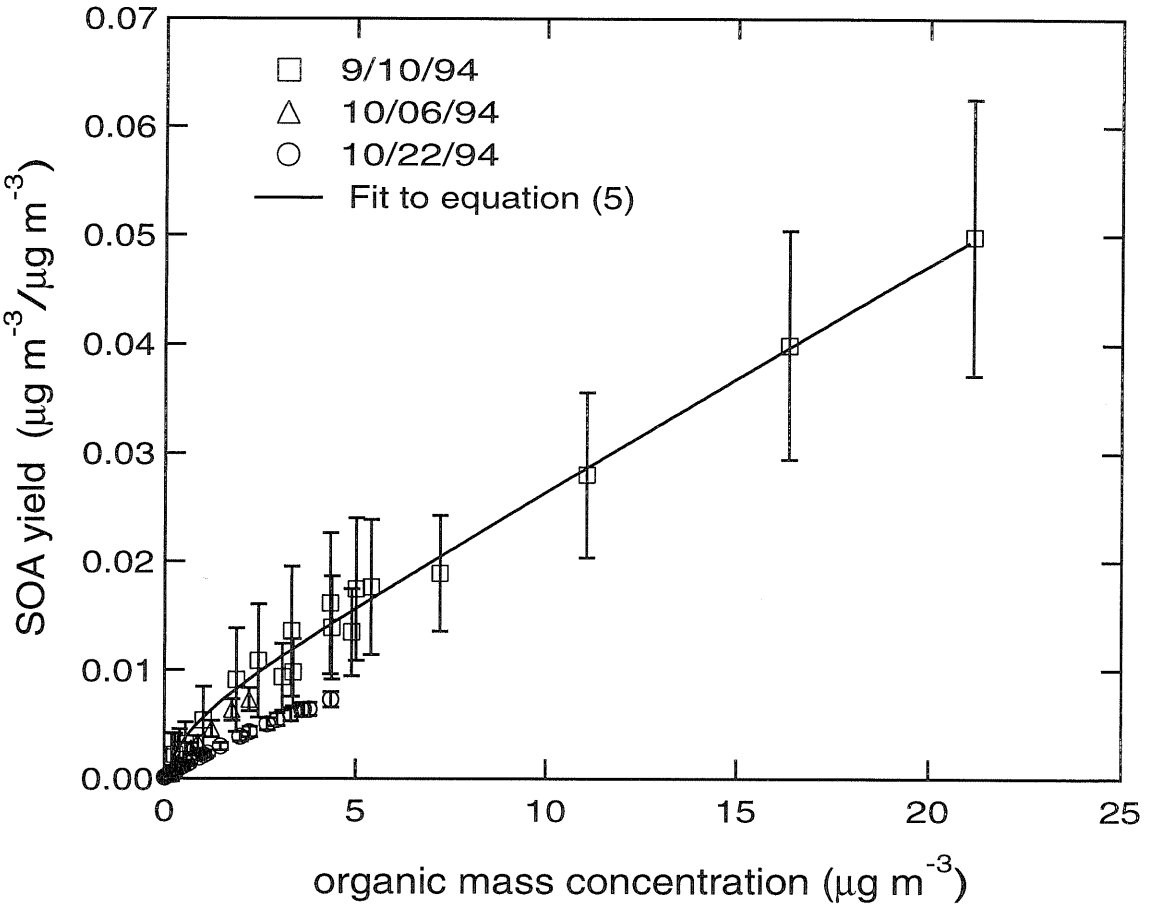

Figure 2.4. Time dependent SOA yields of individual *m*-ethyltoluene experiments as a function of $M_O(t)$. Equation (5) was fitted to the data using a two-product model. Dates of experiments indicated (see Table 2.2).

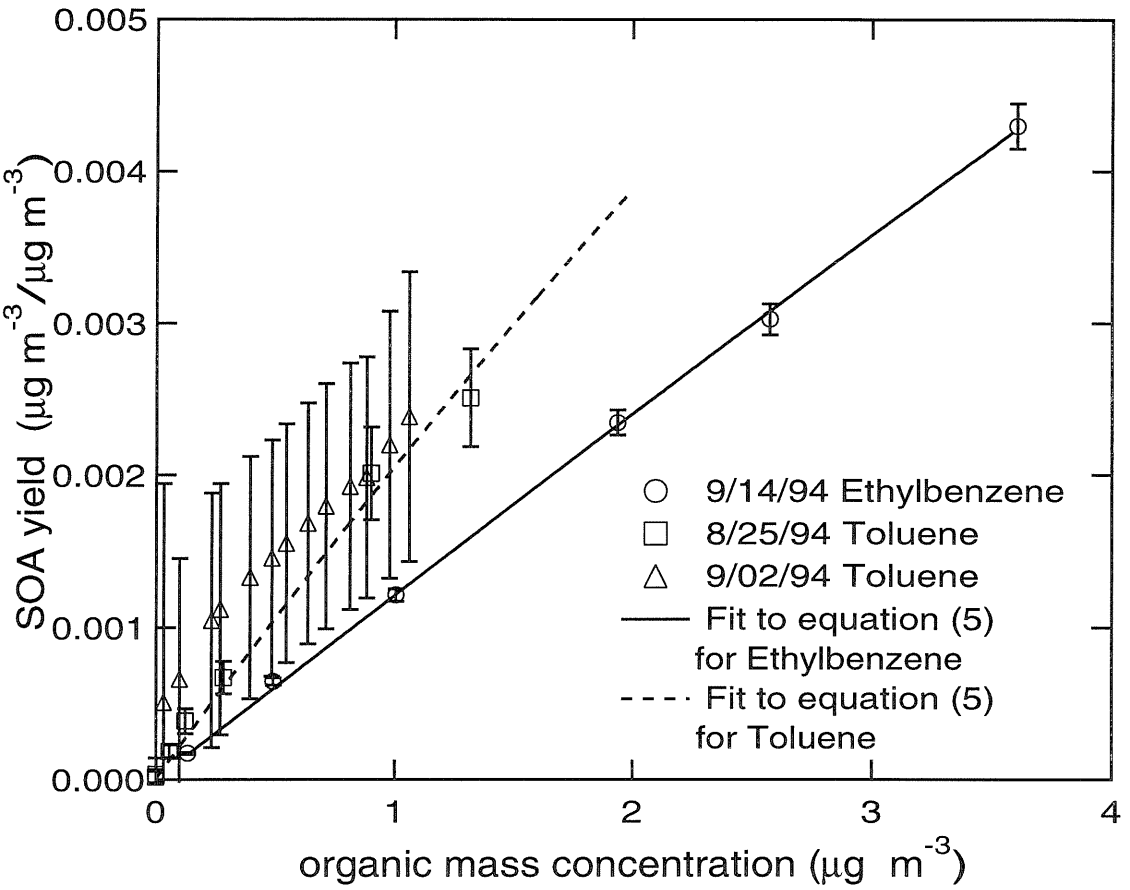

Figure 2.5. Time dependent SOA yields of individual ethylbenzene and toluene experiments as a function of $M_O(t)$. Equation (5) was fitted to the data using a two-product model. Dates of experiments indicated (see Table 2.2).

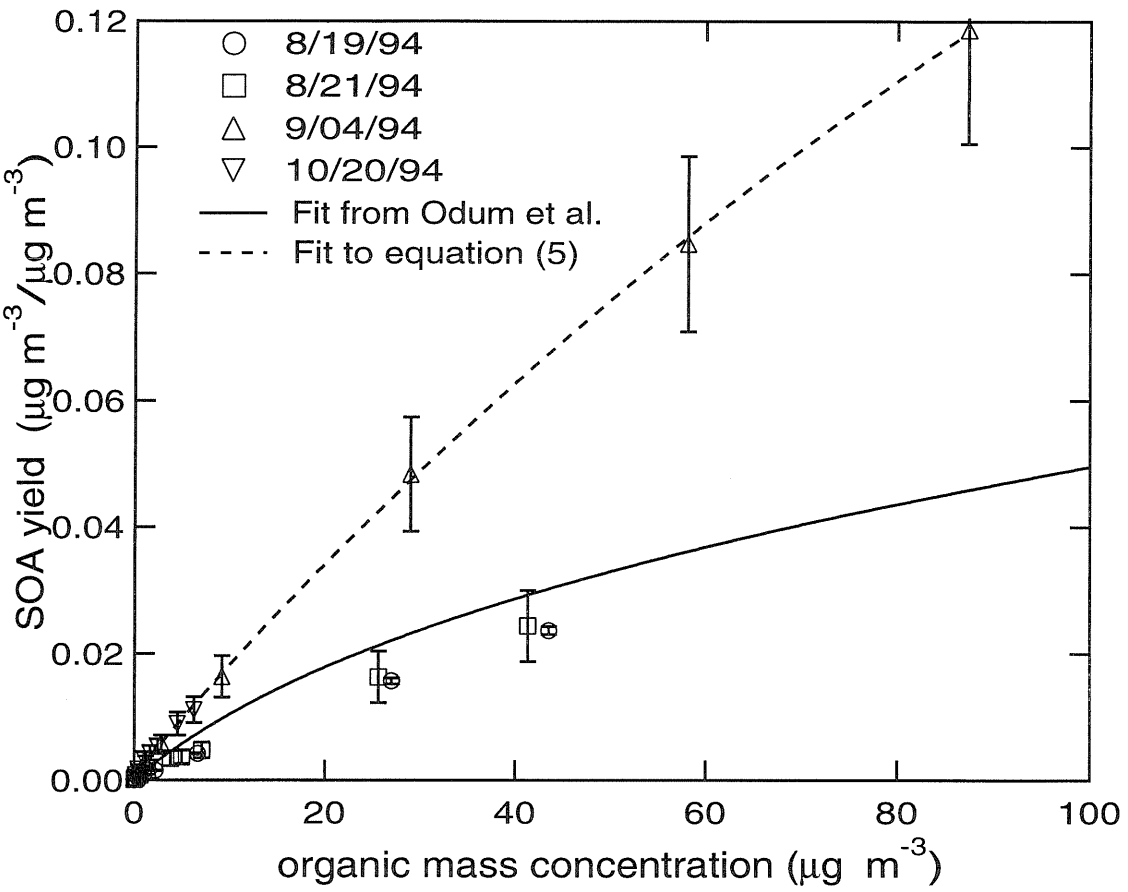

Figure 2.6. Time dependent SOA yields of individual *m*-xylene experiments as a function of $M_O(t)$. The fit from Odum *et al.* (1996) is included. Dates of experiments indicated (see Table 2.2).

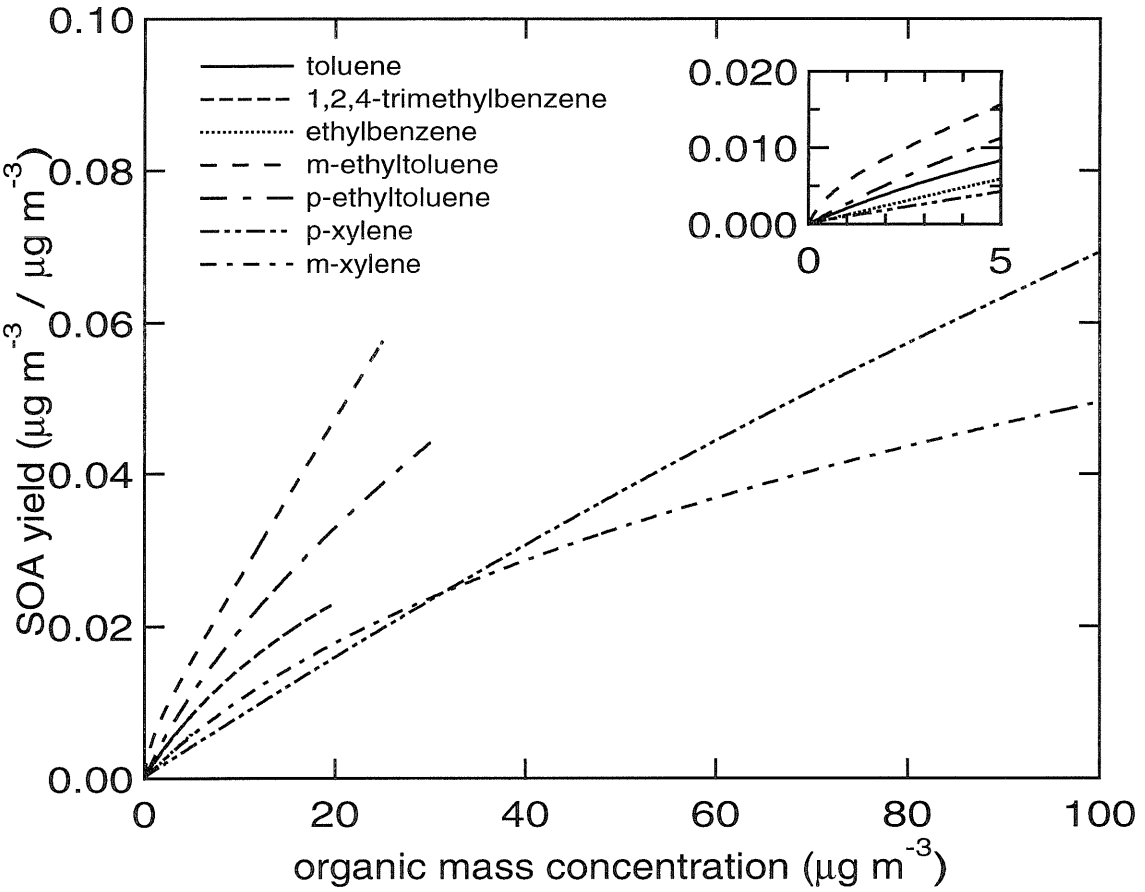

Figure 2.7. Best fits of correlations of yield with organic mass concentration for all aromatics.

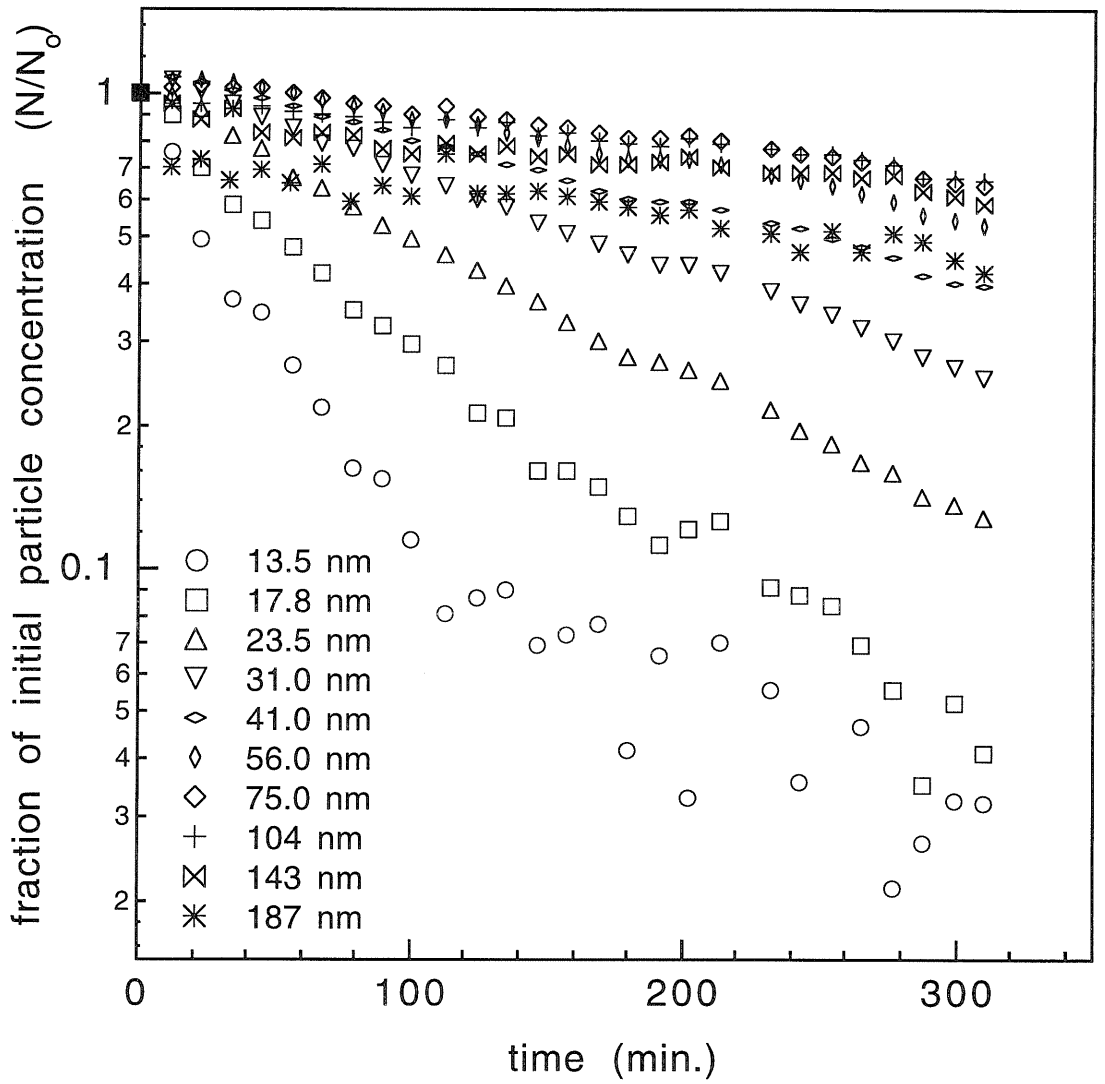

Figure 2.8. Deposition rate of particles expressed as a fraction of the initial particle concentration varying with time.

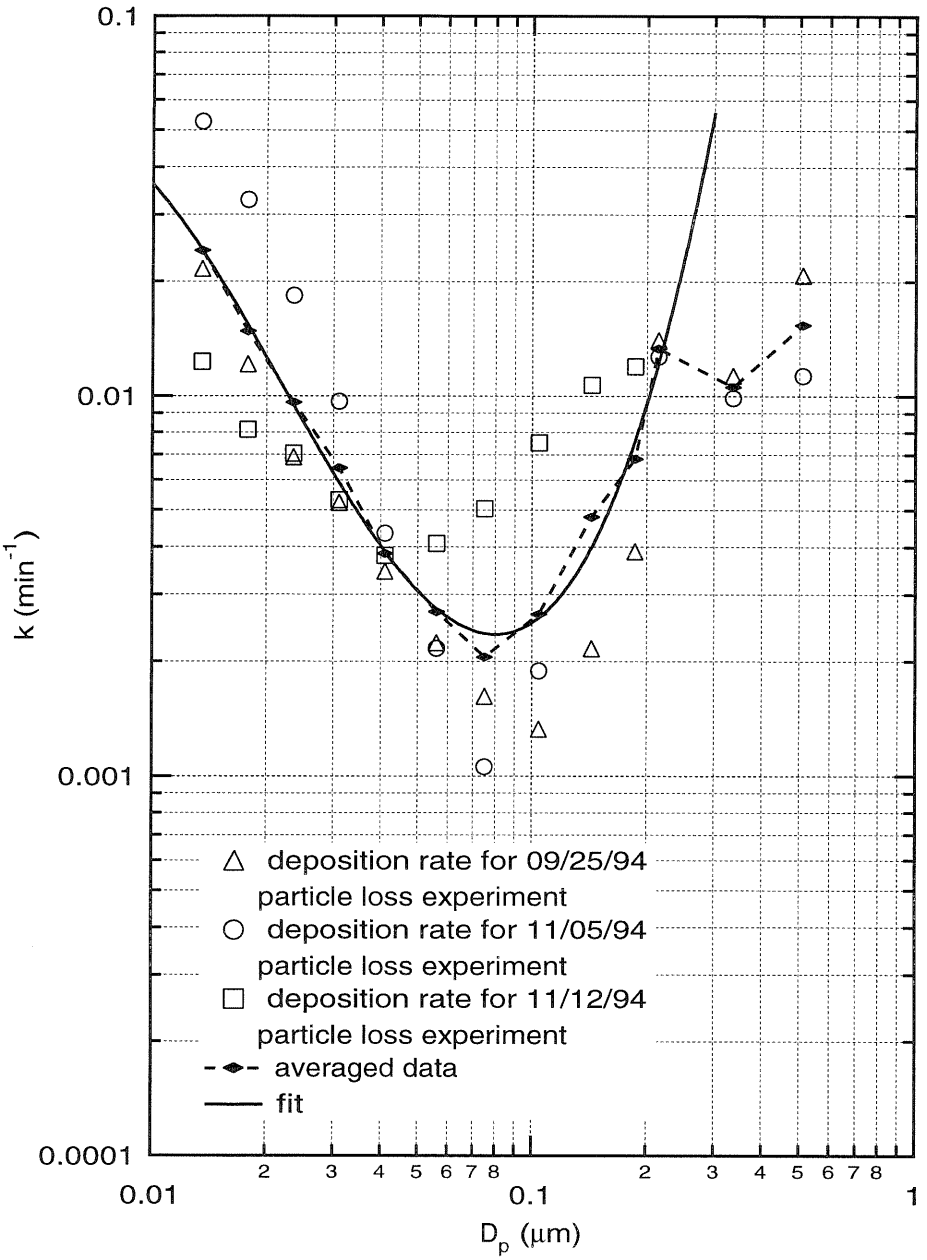

Figure 2.9. Deposition rate as a function of particle size.

Table 2.1. Summary of literature on aerosol yields of aromatic precursors.[a]

AROMATICS	AEROSOL YIELD[b] (%)	FAC[c] (%)	SOURCE
benzene	0	0	(Izumi and Fukuyama, 1990)
toluene	37[d]	1.0-3.0	(Grosjean *et al.*, 1978)
	2-6[e]	0.6-1.4	(Leone *et al.*, 1985)
	4.8[f]	2.1	(Stern *et al.*, 1987)
	1.4-6.2[e]	0.5-1.7	(Gery *et al.*, 1985)
	3.0[g]	2.3	(Izumi and Fukuyama, 1990)
	18.6[f]	6.4	(Wang *et al.*, 1992)
m-, *o*-, *p*-ethyltoluene	3.7, 3.3, 1.5	1.9, 1.4, 0.6	(Izumi and Fukuyama, 1990)
o-xylene	8[d]	6.2	(O'Brien *et al.*, 1975)
m-xylene	3.5	2.9	(Stern *et al.*, 1987)
m-, *o*-, *p*-xylene	2.4-2.6, 2.7, 0.95	2.5-3.1, 2.1, 0.73	(Izumi and Fukuyama, 1990)
ethylbenzene	1.9	0.6	(Stern *et al.*, 1987)
	1	0.78	(O'Brien *et al.*, 1975)
	3.1	2.0	(Izumi and Fukuyama, 1990)
n-propylbenzene	0.98	0.2	(Izumi and Fukuyama, 1990)
isopropylbenzene	2.3	1.0	(Izumi and Fukuyama, 1990)
1,2,3-trimethylbenzene	2.2	1.4	(Izumi and Fukuyama, 1990)
1,2,4-trimethylbenzene	1.1	0.6	(Izumi and Fukuyama, 1990)
1,3,5-trimethylbenzene	1.8	1.2	(Izumi and Fukuyama, 1990)
	2.4	2.1	(Stern *et al.*, 1987)
	0.5-14	0.69-1.92	(O'Brien *et al.*, 1975)
o-cresol	5.1-44.5[h]	0.5-14.0	(Grosjean, 1985)
4-hydroxy-2-nitrotoluene	57	8.6	(Grosjean, 1985)
styrene	0.3	0.5	(Izumi and Fukuyama, 1990)
α-, β-methylstyrene	0.7-4.9, 0.57	1.3-7.6, 1.0	(Izumi and Fukuyama, 1990)
methoxybenzene	2.7	0.8	(Izumi and Fukuyama, 1990)

[a] This table is an updated version of the literature summary found in Grosjean and Seinfeld (1989).

[b] Aerosol yield as reported in the literature for the aerosol formation from the photooxidation of the precursor in the presence of NO_x.

[c] FAC is the fractional aerosol coefficient as defined by Grosjean and Seinfeld (1989). The yields reported in the literature were recalculated according to the conventions and assumptions outlined in the aforementioned paper. The FAC of an aerosol precursor is the ratio of the aerosol ($\mu g\ m^{-3}$) from reactive organic gases to the initial reactive organic gases, also in units of $\mu g\ m^{-3}$. This ratio is expressed as a percentage.

[d] Yield reported as an aerosol light scattering coefficient, b_{scat}, in units of $10^{-4}\ m^{-1}$.

[e] Yield reported as a fraction of the initial carbon present.

[f] Yield reported as defined by equation (1), assuming an aerosol density of 1.0 g cm^{-3}.

[g] Yield reported as defined by equation (2).

[h] Yield reported as defined by equation (1), but assuming an aerosol density of 1.3 g cm^{-3}. Yields also corrected for wall losses.

Table 2.2. Initial conditions of outdoor smog chamber experiments.

aromatic	date	temperature	initial [HC]	initial [C_3H_6]	initial [NO]	initial [NO_2]	initial HC/NO_x ratio	initial particles	peak [O_3]
		°C	ppb	ppb	ppb	ppb	ppbC/ppb	cm^{-3}	ppb
toluene	0819b	35-37	163	---	403	199	2.6	880	595
	0825b	34-38	377	139	431	184	5.0	185	487
	0902b	35-39	558	186	446	256	6.5	2000	314
	0930b	28-30	297	160	393	161	4.6	10420	425
m-xylene	0819a	35-37	740	---	438	216	11.2	745	1140
	0821a	38-40	648	122	375	189	9.8	2600	1092
	0904a	35-38	565	190	328	142	10.8	3250	945
	1020a	23-26	388	284	353	178	7.5	13000	784
	1109b	18-22	860	152	377	191	13.8	2150	400
p-xylene	0821b	36-40	471	156	381	185	7.5	1400	826
	0823b	34-38	442	105	367	164	7.3	1360	756
	0908a	31-36	1082	223	393	255	14.9	2290	868
	0912a	35-39	414	140	349	146	7.5	2000	510
	0921a	24-29	547	299	368	193	9.4	3500	500
ethylbenzene	0825a	34-37	468	112	411	179	6.9	220	256
	0827a	35-38	171	228	549	227	2.6	3300	316
	0906b	32-36	246	176	373	197	6.5	2270	653
	0912b	35-39	326	138	346	141	6.2	1800	168
	0914a	33-36	272	159	336	183	5.1	4530	520
m-ethyltoluene	0906a	32-37	258	196	372	186	5.2	2800	1034
	0910b	34-36	220	219	379	186	4.7	2180	935
	0919b	29-32	437	43	424	192	7.3	1250	788
	1006a	32-35	193	184	373	180	4.1	4330	850
	1020b	22-26	187	282	321	174	5.1	2520	647
	1022a	18-30	419	77	337	188	4.8	1800	419
	1104a	18-24	434	165	367	191	7.9	2950	666
p-ethyltoluene	0829b	35-38	229	242	521	250	3.6	2500	807
	0902a	35-39	270	212	508	284	4.0	760	649
	0910a	34-36	423	204	358	203	7.0	2750	667
	1010b	26-30	279	223	357	172	6.4	4380	650
	1101a	20-29	271	451	367	186	6.9	1360	316
1,2,4-trimethyl-	0827b	35-38	215	214	486	193	3.8	5500	1362
benzene	0904b	35-38	310	201	384	188	5.9	4500	1120
	0916b	30-37	263	222	430	223	4.6	2630	1037
	0921b	24-29	220	275	424	195	4.8	2100	950
	1006b	32-35	437	170	400	185	8.0	2790	950
	1016a	27-30	511	304	438	220	8.5	4080	936
	1016b	27-30	420	258	407	203	9.1	2300	922
	1018b	26-29	522	293	405	203	9.2	4347	927
	1030b	20-25	450	175	332	173	9.1	4910	696

Table 2.3. Densities and molecular weights of typical compounds in secondary organic aerosol.

Compound in SOA[a]	molecular weight g mol^{-1}	density g cm^{-3}
2,5-furandione	98.06	1.31
2,5-hexanedione	114.14	0.97
3'-methylacetophenone	134.18	0.99
3-ethylbenzoic acid	150.18	1.04
3-methyl-2,5-furandione	112.08	1.25
4'-methylacetophenone	134.18	1.01
acetophenone	120.15	1.03
benzaldehyde	106.12	1.04
benzoic acid	122.13	1.27
dihydro-2,5-furandione	100.08	1.23
dihydro-5-methyl-2(3H)-furanone	100.12	1.06
m-tolualdehyde	120.15	1.02
m-toluic acid	136.15	1.06
p-tolualdehyde	120.15	1.02

[a]Refer to Forstner *et al.* (1996) for a complete list of the species identified in aromatic secondary organic aerosol.

Table 2.4. Parameters of fits to equation (5).

aromatic	α_1 ($\mu g\ m^{-3}/\mu g\ m^{-3}$)	K^1_{om} ($m^3\ \mu g^{-1}$)	α_2 ($\mu g\ m^{-3}/\mu g\ m^{-3}$)	K^2_{om} ($m^3\ \mu g^{-1}$)
p-ethyltoluene	0.164	0.0977	0.291	0.00410
p-xylene				
8/23/94	0.000785	2.524	0.809	0.00204
8/21/94 + 9/08/94	0.000212	14.5	0.447	0.00183
m-ethyltoluene	0.00591	1.41	4.73	0.000443
m-xylene				
(Odum *et al.*, 1996)	0.03	0.032	0.167	0.0019
9/4/94	0.00182	0.300	0.499	0.00349
1,2,4-trimethylbenzene				
(Odum *et al.*, 1996)	0.0324	0.053	0.166	0.002
toluene	0.0348	0.0627	0.000585	0.0000657
ethylbenzene	0.0219	0.0170	0.273	0.00311

CHAPTER 3

Secondary Organic Aerosol from the Photooxidation of Aromatic Hydrocarbons: II. Molecular Composition

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Abstract

Outdoor smog chamber photooxidations to determine the molecular composition of secondary organic aerosol (SOA) from toluene, *m*-xylene, *p*-xylene, ethylbenzene, *m*-ethyltoluene, *p*-ethyltoluene, and 1,2,4-trimethylbenzene in sunlight-irradiated hydrocarbon-NO_X mixtures are reported. Gas-phase mechanisms leading to the observed products are proposed. Unsaturated anhydrides (2,5-furandione, 3-methyl-2,5-furandione, 3-ethyl-2,5-furandione) are predominant components of aerosol from all the aromatics, an observation that is consistent with gas-phase aromatic mechanisms involving ring-fragmentation. Saturated anhydrides were also detected in significant quantities, which could result from the hydrogenation of the furandiones in sunlight in the particle phase.

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Introduction

Hydrocarbons are emitted to the troposphere from anthropogenic and biogenic sources. Anthropogenic sources comprise organics such as alkanes, alkenes, aromatics, and carbonyls, while biogenic sources include organics such as terpenes and sesquiterpenes. The atmospheric photooxidation of organics yields oxygenated and nitrated products that, depending on their properties, partition between the gas and particulate phases, resulting in secondary organic aerosol (SOA) formation. The atmospheric chemistry of larger organic compounds is sufficiently complex that a spectrum of condensable and non-condensable products form from a single hydrocarbon precursor. The recent work of Pankow (1994ab) on semi-volatile organic gas/particle partitioning theory and the experimental evidence of Odum *et al.* (1996) and Forstner (1996) establishes that vapor pressure alone does not determine to what extent a vapor species will partition into the particle phase. The organic particulate mass serves as the medium into which the gas-phase species are absorbed, and thereby the amount of organic particulate mass directly affects the gas/particle partitioning. A consequence of this is that products with relatively high vapor pressures may well exist, in part, in the particle phase.

Aromatics are particularly important constituents of urban and regional atmospheric chemistry (Lurmann and Main, 1992); additionally, most have been identified as aerosol precursors (Stern *et al.*, 1987; Wang *et al.*, 1992; Izumi and Fukuyama, 1990; Odum *et al.*, 1996; Forstner, 1996). Although the initial reactions of aromatics with OH are reasonably well understood, those beyond the first few steps in the NO_X-air photooxidation remain uncertain (Atkinson, 1994). Typically, less than 50% of the reacted carbon has been identified in photooxidation product studies of toluene, *p*-xylene, and *m*-xylene (Atkinson, 1994). Elucidation of the photooxidation mechanisms of aromatics remains crucial for understanding their contribution to ozone and other oxidized product formation and to eventual formation of SOA (National Research Council, 1991). Although the focus of this

work was the composition of secondary organic particulates, it confirms first generation product identification (Atkinson, 1994), and in particular it corroborates the identification of dicarbonyls and anhydrides (Bierbach *et al.*, 1994). Additional new product information for two aromatics, ethylbenzene and *p*-ethyltoluene has been obtained. Finally, the original identification of saturated anhydrides from some aromatic precursors is suggestive of photochemically-driven particle-phase hydrogenation.

The present study represents a comprehensive effort to determine the composition of aromatic secondary particulates. The goals are to assess aromatic photooxidation mechanisms by identifying particle-phase products, and to obtain molecular product information allowing future development of quantitative prediction of SOA formation. Few studies have attempted to systematically identify components of secondary organic particulates. The current study has identified species in aromatic secondary aerosol, thereby providing compelling evidence for the semi-volatile organic gas/particle partitioning theory of Pankow (1994ab). The identified species in the secondary organic particulates have high vapor pressures, such that condensation as the mechanism to the particle phase is precluded. A logical mechanism by which these species can exist in the particle phase is the establishment of an equilibrium between the gas-phase concentration and the particulate organic mass concentration.

A series of outdoor smog chamber aromatic-NO_X photooxidations were performed to generate secondary organic aerosol. The aromatics studied were toluene, *m*-xylene, *p*-xylene, ethylbenzene, *m*-ethyltoluene, *p*-ethyltoluene, and 1,2,4-trimethylbenzene. After a description of the experiments and the analytical method, we summarize the species identified in the secondary organic particulates from the above aromatics and discuss mechanisms leading to these products.

Experimental

Secondary Organic Aerosol Sample Generation. The 60 m^3 outdoor smog chamber facility has been described previously (Wang *et al.*, 1992; Forstner, 1996; Odum *et al.*, 1996). Experiments were performed over the summers of 1993 and 1994. A summary of experiments performed in 1994 is given in Forstner (1996). Initial hydrocarbon mixing ratios ranged from 200 to 900 ppb, and initial propene mixing ratios ranged from 100 to 340 ppb. Propene was added to the mixture to enhance photochemical reactivity (Wang *et al.*, 1992). Initial hydrocarbon-NO_X ratios ranged from 3 to 14 ppbC/ppb, similar to those observed in the South Coast Air Basin of California (Lurmann and Main, 1992). Ammonium sulfate seed aerosol was added to encourage condensation of the secondary gas-phase products. In the 1993 experiments, an 8 m^3 outdoor Teflon chamber was used (Table 3.1). Initial hydrocarbon mixing ratios ranged from 2 to 8 ppm, and initial propene mixing ratios were approximately 1 ppm. Hydrocarbon-NO_X ratios were at least 25 ppmC/ppm, a level that has been previously found to be optimal for secondary organic aerosol formation (Zhang *et al.*, 1992). Initial particles were also injected into the small smog chamber at concentrations up to 1000 cm^{-3}. It is important to note that, although the initial individual hydrocarbon concentrations are an order of magnitude or more above ambient urban levels, the hydroxyl radical chemistry occurring in the chamber is the same as that under ambient conditions. Hence, these mechanistic observations are expected to be valid for atmospheric conditions. The subsequent reactions of the OH-aromatic adducts are not independent of NO_2 concentrations, and in consideration of the high NO_2 levels in smog chamber experiments compared to ambient conditions, these OH-aromatic adduct reactions are significant than in the ambient atmosphere.

Sample Collection. Once significant secondary particulate matter had formed, as monitored by the Scanning Electrical Mobility Spectrometer (Wang and Flagan, 1990),

particles were collected. Sampling typically began four to six hours into the experiment. The smog chamber was deflated through filter samplers, each operating at 10 L min^{-1}. For the experiments, five samplers all containing quartz fiber filters were used. Quartz fiber filters 47 mm in diameter from Pallflex (Putnam, CT) were used. Sampling lasted from two to four hours. Prior to usage, the filters were baked at 750°C for at least 2 h. The filters were stored in glass jars with Teflon-lined lids at sub-zero temperatures immediately after collection. The storage jars were prepared prior to use by rinsing in distilled water, then twice with HPLC-grade methanol, and finally in HPLC-grade methylene chloride. The open ends of the jars were covered with foil and the jars were baked at 550°C for at least 4 h. The filter samplers and the Teflon-lined lids of the jars were similarly cleaned by sonication in distilled water, then in HPLC-grade methanol, and finally in HPLC-grade hexane. The sample collection procedure and the cleaning protocol with respect to handling quartz fiber filters has been adapted from the procedure of Hildemann *et al.* (1991) and Rogge *et al.* (1991; 1993abcd).

Various blank filters were tested for quality assurance. One test involved extracting filters immediately after baking at 750°C. The extraction procedure is outlined in the following section. The filters were found to contain no trace organics. Filter samples were also taken from the smog chamber on those days during which the chamber was baking. These filters of background particle loading contained trace amounts of organics, potentially identifiable as isobenzofurandione and phthalide. Phthalates are common plasticizers and are often detected as contaminants in sampling studies (Rogge *et al.*, 1991). It should be noted that organic vapors may absorb onto particles already collected on the filter surface. This aspect was not quantified in the present study. Compounds that are particle-bound during sampling are considered to comprise the collected aerosol in primary aerosol studies (Rogge *et al.*, 1991, 1993abcd). This lack of quantification was not viewed as critical to the goal of this study of identifying organic products that are susceptible to

partitioning to the particle phase. By identifying the organics, we can evaluate chemical mechanisms leading to these species. For further reference in this paper, the species identified from the extraction of particulates and absorbed organic vapors on quartz fiber filters, are correctly referred to as species of secondary organic aerosol.

Sample Extraction. A new extraction protocol was developed for the quantitative analysis of secondary organic aerosol on quartz fiber filters (Forstner *et al.*, 1996). The extraction method was optimized by recovery studies of filters impregnated with 5 to 50 μl of an organic standard containing an approximate concentration each of 1 mg μl^{-1} in methanol: *t*-butyl hydroperoxide, butyl ester of nitric acid, heptanal, hexanoic acid, nonanal, 2-ethylhexyl nitrate, 2-nitro-*m*-xylene, benzoic acid, 5-nitro-*m*-xylene, undecanal, decanoic acid, pentanedioic acid, hexanedioic acid, dodecanoic acid, and tetradecanoic acid (Forstner *et al.*, 1996). These compounds were chosen as they have either been previously identified as gas-phase oxidation products (Paulson and Seinfeld, 1992; Atkinson, 1994) or they have relevant functional groups, for example, nitrates and hydroperoxides. Numerous extractions of the recovery standard were performed and no conversion of any of the species in the standard were observed. The SFE-GC/MS (supercritical fluid extraction-gas chromatograph/mass spectrometer) system does not appear to induce any reaction of the analytes. The optimal method was found to be extraction using supercritical CO_2, modified with a 10% solution of acetic acid in methanol. The addition of acetic acid was necessary for extraction of organic acids from the quartz fiber filters. The Suprex PrepMaster (Pittsburgh, PA) extraction unit and modifier pump were used. The filters were allowed to equilibrate in CO_2 at 150 °C and 420 atm for 10 min. Then the filters were extracted for 30 min with CO_2 flowing at approximately 1 ml min^{-1}. Modifier was added at a rate of 2% of the CO_2 flow rate. Analytes and CO_2 passed directly through a heated transfer line to the gas chromatograph (GC). The GC column was cryo-cooled to -30 °C,

trapping the analytes in the first few meters of the column while allowing the CO_2 to vent. Once the extraction was complete, the GC stepped through its temperature program.

GC/MS Analysis. A Hewlett Packard 5890 Series II gas chromatograph and a Hewlett Packard 5989A mass spectrometer engine were used. After high resolution chromatography using an HP-1701 60m fused silica column (14% cyanopropyl-phenyl methyl-polysiloxane) with a film thickness of 0.25 μm and inner diameter of 0.25 mm, the MS analyses were performed by electron impact ionization. The HP ChemSystem software in conjunction with the Wiley library of organic spectra was employed to initially identify organic compounds in the samples. The species identified were later confirmed by matching retention times with authentic standards and then quantified. All standards were obtained from Aldrich Chemical Co. (St. Louis, MO) and were used without further purification.

Composition of Secondary Organic Aerosol

The compounds identified are listed alphabetically in Table 3.2 for all aromatic systems. The quantities measured for each compound have been normalized with respect to the total mass of identifiable species from the parent hydrocarbon. Only 15 to 30% of the mass which was extracted from the quartz filters and eluted through the gas chromatograph, could be verified with standards. This result is typical of molecular composition studies of complex atmospheric aerosol mixtures (Rogge *et al.*, 1991, 1993abcd). The unidentified fraction consists of peaks that are not specifically identifiable and the unresolved mixture emerging late in the chromatograms. The entries in Table 3.2 are normalized amounts expressed as a percentage; they reflect the relative contribution each compound makes to the quantifiable and identifiable SOA for the particular parent aromatic. Species detected but at a level too low to be quantified are denoted with '+.' All species, except when noted, were verified and quantified with authentic standards. The remaining compounds were

tentatively identified either with a match in a mass spectral library or by interpretation of the mass spectra. Contributions of these organics to the identifiable SOA were estimated from the response of similarly structured compounds, as noted in the footnotes to Table 3.2.

The distribution of products in the secondary organic aerosol reflects the results of two distinct processes: the gas-phase photooxidation of the aromatic and the subsequent partitioning of the reaction products into the particle phase. Firstly, there is a gas-phase yield associated with each first-, second-, third-, *etc.* generation product according to the oxidation chemistry resulting in its formation. As an example, consider benzaldehyde. Toluene reacts with OH radicals, with a benzaldehyde yield of approximately 10% (Atkinson, 1994). That is, for every 10 molecules of toluene that reacts with OH in the presence of sufficient NO_X, one molecule of benzaldehyde forms. Then there is another yield, or more precisely a gas/particle partitioning, associated with the benzaldehyde molecule. This partitioning may depend on physico-chemical parameters, such as the compound's vapor pressure, the amount of organic aerosol present, and temperature. The overall measured contribution of a product like benzaldehyde to the measured aerosol mass reflects both its gas-phase reaction yield and its gas/particle partitioning coefficient. The aerosol mass which is identified is typically less than 1% of the total amount of reacted aromatic. Consequently, an attempt to interpret the results in Table 3.2 as gas-phase reaction yields is inappropriate.

Toluene. The toluene-OH reaction results in about 10% H-atom abstraction from the methyl group and 90% OH addition to the ring (Atkinson, 1994). The addition pathway is thought to yield ring-fragmentation products, in amounts upwards of 65% of the overall OH radical reaction (Atkinson, 1994). The components of toluene SOA identified and verified in the present study comprise less than 40% ring-retaining products, and more than 60% of those most likely arising from ring-fragmentation pathways. The more dominant identified species in toluene SOA include 3-methyl-2,5-furandione,

dihydro-2,5-furandione, 2-methyl-4-nitrophenol, 2,5-furandione, 3-methyl-4-nitrophenol, and benzoic acid. Mechanisms leading to the formation of these compounds will be discussed subsequently. The presence of relatively high vapor pressure ring fragmentation products in SOA is consistent with the semi-volatile gas/particle partitioning model in which gas-phase organics absorb into the organic particulate phase (Pankow, 1994ab; Odum *et al.*, 1996; Forstner, 1996). The predominant compound identified in toluene SOA is 3-methyl-2,5-furandione, also known as citraconic anhydride, the anhydride of citraconic acid. This compound has estimated vapor pressures of 1 mmHg (1320 ppm) and 5 mmHg (6580 ppm) at 47.1°C and 74.8°C, respectively (Jordan, 1954). If vapor pressure alone determines whether or not a compound is present in the particle phase, it would not be expected that 3-methyl-2,5-furandione would be an aerosol component. Another example is 2,5-furandione of which a significant amount is in the particle phase, yet its vapor pressure has been estimated to be 0.36 mmHg (470 ppm) at 35°C (Jordan, 1954). According to the gas/particle partitioning model, in order for either of these compounds to exist in the particle phase they must absorb into the organic aerosol mass. Although the presence of these anhydrides could also result from the dehydration upon heating of the corresponding dicarboxylic acids (Streitwieser and Heathcock, 1976), for example, 3-methyl-2,5-furandione from citraconic acid, during supercritical CO_2 extraction, adipic acid and glutaric acid were included in the standard and no cyclization of these compounds was detected. Furthermore, since the relative humidity of the smog chamber experiments ranged from 15 to 25%, conversion of the anhydride to the corresponding acid is unlikely. The presence of these anhydrides arises largely from gas/particle partitioning.

***m*-Xylene.** Ring-fragmentation products comprise a significant portion (approximately 75%) of the SOA, with the remainder ring-retaining products. Dominant organics in the total identifiable mass include 3-methyl-2,5-furandione, *m*-toluic acid, and 2,5-furandione.

***p*-Xylene.** Organics contributing primarily to the identifiable SOA are 3-methyl-2,5-furandione, *p*-tolualdehyde, 4-methyl-2-nitrophenol, 2,5-hexanedione, dihydro-2,5-furandione, and *p*-toluic acid. The contribution of 4-methyl-2-nitrophenol to SOA is uncertain, as there is significant error (>100%) in the measurement (Table 3.2.) It is likely that artifact in one sample (of four taken) skewed the calculation of the average distribution. Hence, 4-methyl-2-nitrophenol is interpreted as a contaminant from a previous experiment.

1,2,4-Trimethylbenzene. Nearly an equal split between ring-retaining and ring-fragmentation products were identified in 1,2,4-trimethylbenzene SOA. The organics contributing significantly (greater than 5% by mass) to the identifiable SOA include 4-methylphthalic acid, 3-methyl-2,5-furandione, 3,4-dimethylbenzoic acid, 3-methyl-2,5-hexanedione, and 2,5-furandione. It should be noted that 3-methyl-2,5-hexanedione was not verified with an authentic standard, but was only identified from a match with a library entry. Consequently, its identification should be viewed as provisional until verification.

Ethylbenzene. A significant portion of the organics identified likely arise from ring-fragmentation mechanisms. The species identified in decreasing order of significance are acetophenone, 3-methyl-2,5-furandione, 2,5-furandione, dihydro-5-methyl-2-furanone, benzaldehyde, 3-ethyl-2,5-furandione, and an ethyl-nitrophenol. It should be noted that 3-ethyl-2,5-furandione and the ethyl-nitrophenol were not verified with authentic standards, but were only identified from matches with library entries.

***m*-Ethyltoluene.** Species contributing over 5% of the SOA mass are 3-ethyl-2,5-furandione, 3-methyl-2,5-furandione, 3'-methylacetophenone, 2,5-furandione, 3-ethylbenzoic acid, *m*-tolualdehyde, and dihydro-2,5-furandione.

***p*-Ethyltoluene.** Species contributing over 5% of the SOA mass are 3-ethyl-2,5-furandione, 3-methyl-2,5-furandione, 4'-methylacetophenone, *p*-tolualdehyde, and 2,5-furandione.

Toluene Photooxidation Mechanisms

Possible mechanisms leading to the toluene-OH radical products identified as SOA components are depicted in Figures 1-5. The species listed in Table 3.2 identified in the aerosol phase are highlighted in the mechanisms by boxes. Only mechanisms of toluene photooxidation leading to the more predominant products will be discussed. The initial OH radical attack on toluene is depicted in Figure 3.1, illustrating the abstraction/addition pathway split and, as noted above, the formation of benzaldehyde (Atkinson, 1994), which can further oxidize to benzoic acid. OH abstracts a hydrogen atom from the carbonyl group, and oxygen adds to the radical. This peroxy radical can react with RO_2 (or HO_2) to form the carboxylic acid directly, or it can react with NO to form an alkoxy radical and NO_2. The alkoxy radical can abstract a hydrogen from another toluene molecule, benzaldehyde molecule, or from a formaldehyde molecule, to yield the carboxylic acid and to propagate the radical chain reaction. Figure 3.1 also outlines this suggested mechanism leading to the acid.

The addition of OH to the ring results in methyl-hydroxycyclohexadienyl radicals (Figure 3.1), a path estimated to be 90% of the OH-toluene reaction. Most products in toluene photooxidation result from subsequent reactions of the methyl-hydroxycyclohexadienyl radical, comprising both ring-retaining species and ring-fragmentation species. The OH radical can add to toluene in the *ortho-*, *meta-* and *para-*

positions, with the *ortho-* position energetically favored (Andino *et al.*, 1996). The methyl-hydroxycyclohexadienyl radical may react with O_2 or NO_2 (Atkinson, 1994; Bierbach *et al.*, 1994; Goumri *et al.*, 1990, 1991; Andino *et al.*, 1996).

The methyl-hydroxycyclohexadienyl radical reacts with O_2 to form a methyl-hydroxycyclohexadienyl peroxy radical (Figure 3.2). OH is favored thermodynamically to add *ortho* to the methyl group on the ring, and the peroxy group can bridge as shown in Figure 3.2 (Jeffries *et al.*, 1995; Andino *et al.*, 1996). The resulting alkyl radical rapidly adds O_2 and reacts with NO to form NO_2 and an alkoxy radical. This alkoxy radical decomposes to form either *cis-* or *trans*-butenedial, and an oxo-hydroxypropyl radical. *trans*-Butenedial has been shown to photoisomerize to *cis*-butenedial with a rate constant of $3.9\pm0.3\text{x}10^{-4}$ s^{-1} (Bierbach *et al.*, 1994). The *cis-* isomer has been postulated to lose a hydrogen atom from the carbonyl group via OH radical attack or by photolysis, with subsequent O_2 addition and rearrangement to form 2,5-furandione (Bierbach *et al.*, 1994). The details of this mechanism are outlined in Figure 3.2.

Of the identifiable fraction of toluene SOA, 3-methyl-2,5-furandione is the predominant species. Based on the photoisomerization and oxidation mechanism for unsaturated dicarbonyls proposed by Bierbach *et al.* (1994), the formation of 3-methyl-2,5-furandione is consistent with that from 2-methyl-2-butenedial. Figure 3.3a shows the detailed mechanism to form this anhydride from the unsaturated dicarbonyl, in addition to the rearrangement mechanism to form 3-methyl-2(5H)-furanone. Mechanisms to form 2-methyl-2-butenedial from OH-toluene adducts are outlined in Figure 3.3b and 3.3c. The more likely mechanism arises from the energetically favored *ortho*-methyl-hydroxycyclohexadienyl radical (Figure 3.3b). After the addition of oxygen, this radical cleaves to form 2-methyl-2,4-hexadienedial (Hoshino *et al.*, 1978; Bartolotti and Edney, 1995). Addition of hydroxyl radicals results in 2-methyl-2-butenedial. The other mechanism involves OH radical addition to toluene in the *meta-* or *para* positions with

further oxidation leading to a bridged peroxy alkyl radical (Figure 3.3c). This alkyl radical can be further oxidized and ultimately fragment to form 2-methyl-butenedial and an oxygenated ethyl radical (Andino *et al.*, 1996).

Significant quantities of dihydro-2,5-furandione (succinic anhydride) were detected in the toluene aerosol (Table 3.2). Upon first consideration it would seem that a saturated anhydride would not result from the photooxidation of an aromatic compound, particularly since previous studies have not reported saturated compounds. Photoreduction of ketones in the solution phase is well established, and there is evidence to support intermolecular hydrogen abstraction of cyclic ethylenes after photo-excitation (Turro, 1978). Given the lack of prior evidence of succinic anhydride as a product in gas-phase toluene photooxidation, it is possible that succinic anhydride forms from the intermolecular hydrogen abstraction of 2,5-furandione in the particle phase. Water, nitrophenols, and benzoic acid, in the particle phase can contribute to a slightly acidic environment in the particle, allowing facile proton (H) exchange. Figure 3.4 outlines a possible mechanism to produce dihydro-2,5-furandione. Once in the particle phase, the 2,5-furandione is photolytically excited and may break one of the double bonds, to make an alkyl bi-radical. Upon interaction with this alkyl bi-radical, water or a nitrophenol will readily yield a hydrogen, resulting in an alkyl radical and a hydroxyl or phenoxy radical. The alkyl radical will abstract another H-atom from another water molecule or nitrophenol molecule to produce succinic anhydride. Because the double bond and di-ketone portion of 2,5-furandione is highly reactive (*cf.* 1,4-benzoquinone), dihydro-2,5-furandione can form.

The methyl-hydroxycyclohexadienyl radical may react with NO_2, particularly in environmental chamber studies where NO_X levels are elevated, to yield the corresponding cresols (Atkinson, 1994). A detailed mechanism for this step is not shown in Figure 3.5. After the methyl-hydroxycyclohexadienyl radical reacts with NO_2 to result in either *o*-, *m*-,

or *p*-cresol, OH can react with the cresol to abstract an H-atom from the hydroxyl group or add to the ring (Atkinson, 1994). Only the abstraction pathway is shown in Figure 3.5. This methyl phenoxy radical can then react with NO_2 to form a variety of nitro methyl phenolic compounds. The positions of —O• and the methyl group determine where NO_2 adds to the ring. Alkyl groups and —OR groups on an aromatic ring are *ortho-* and *para-*directing, with —OR more strongly activating (Streitwieser and Heathcock, 1976). Hence, NO_2 adds *ortho* and *para* to the oxygen in the methyl phenoxy radical. The steps leading to 2-methyl-4-nitrophenol, 3-methyl-4-nitrophenol, and 4-methyl-2-nitrophenol are outlined in Figure 3.5, with these identified toluene SOA products boxed. Also shown in Figure 3.5 are further reactions of 2-nitro-6-methylphenol with OH and NO_2 to yield 2-methyl-4,6-dinitrophenol, another species detected in toluene SOA.

m-Xylene Photooxidation Mechanisms

Three compounds, 3-methyl-2,5-furandione, *m*-toluic acid, and 2,5-furandione, comprise 75% of the identified *m*-xylene SOA. The mechanism leading to *m*-toluic acid is readily extended from the toluene-OH mechanism resulting in benzaldehyde and benzoic acid. The OH abstraction pathway for *m*-xylene is shown in Figure 3.1, with the subsequent steps to the carboxylic acid. On the basis of *ab initio* calculations, Andino *et al.* (1996) determined that OH adds to *m*-xylene in the *ortho* position to both methyl groups, leading to the ring-fragmentation product of 4-oxo-2-pentenal. Less favored is OH-addition in the *para-* and *ortho-* position to both methyl groups and the subsequent oxygen addition and β-scission reaction to yield 2-methyl-2-butenedial and 2-methyl-4-oxo-2-pentenal. Bierbach *et al.* (1994) postulate a mechanism by which 4-oxo-2-pentenal can form 2,5-furandione. This mechanism involves the initial loss of the hydrogen adjacent to the carbonyl group by photolysis or OH abstraction. Subsequent addition of oxygen to the alkyl radical, formation of an alkoxy radical, and cyclization lead to 2,5-furandione (Figure

3.6). The mechanism to yield 3-methyl-2,5-furandione is outlined in Figure 3.3 from the photooisomerization and oxidation of 2-methyl-2-butenedial. Since 3-methyl-2,5-furandione contributes 60% by mass to the SOA, another pathway leading to this compound may exist, in addition to the ring-fragmentation leading to 2-methyl-2-butenedial. Extending the mechanism in Figure 3.6 to 2-methyl-4-oxo-pentenal, another pathway to 3-methyl-2,5-furandione is proposed.

p-Xylene Photooxidation Mechanisms

Similar to toluene and *m*-xylene, OH can either abstract a hydrogen from one of the methyl groups on *p*-xylene or it can add to the ring. The hydrogen abstraction pathway leads to *p*-tolualdehyde, which is identified as a significant constituent of *p*-xylene SOA. Further oxidation of *p*-tolualdehyde leads to the formation of *p*-toluic acid. The OH abstraction pathway is shown in Figure 3.1 resulting in the aldehyde and carboxylic acid. Andino *et al.* (1996) also studied ring-fragmentation products from the bicyclic oxy radicals from *p*-xylene-OH addition. Because of *p*-xylene's symmetry, only 2-methyl-2-butenedial and 3-hexene-2,5-dione result. Again, as described in Figure 3.3 and in the previous sections, 3-methyl-2,5-furandione is formed from the photoisomerization and oxidation of 2-methyl-2-butenedial. As suggested in the toluene mechanism, dihydro-2,5-furandione may arise from a photolytic hydrogenation process of 2,5-furandione in the particle phase. Formation of 2,5-hexanedione can be analogously postulated. The 3-hexene-2,5-dione can partition into the particle phase, and may be photolytically excited to break one bond of the double bond, to produce an alkyl bi-radical. Water, *p*-toluic acid, and nitrophenols, have pK_a values of 14.9, 4.38, and approximately 8 (Streitwieser and Heathcock, 1976). Hence, upon interaction with this alkyl bi-radical, these compounds can yield a hydrogen, resulting in an alkyl radical and a hydroxyl or phenoxy radical. The alkyl radical will abstract another hydrogen from another water molecule or nitrophenol molecule to yield

2,5-hexanedione. This process is outlined in Figure 3.7. The other saturated organic comprising a significant portion of *p*-xylene SOA is dihydro-2,5-furandione. Its origin from 2,5-furandione has been outlined in Figure 3.4. Although Bierbach *et al.* (1994) demonstrated experimentally that 2,5-furandione is produced from the UV photolysis of 3-hexene-2,5-dione, it is unlikely that this reaction occurs in the outdoor smog chamber as the relevant wavelengths are above about 290 nm. The origin of dihydro-2,5-furandione from *p*-xylene photooxidation is presently uncertain, and possibly may arise from the photooxidation of 3-hexene-2,5-dione as shown in Figure 3.8.

1,2,4-Trimethylbenzene Photooxidation Mechanisms

The SOA resulting from 1,2,4-trimethylbenzene photooxidation contains significant amounts of ring-retaining carboxylic acids. 4-Methylphthalic acid and 3,4-dimethylbenzoic acid can result from the atmospheric oxidation of 4-methyl-1,2-benzenedicarboxaldehyde and 3,4-dimethylbenzaldehyde, respectively. The substituted aldehydes arise from an OH abstraction mechanism similar to that depicted in Figure 3.1 for toluene, *m*-xylene, and *p*-xylene. Andino *et al.* (1996) proposed the following gas-phase ring-fragmentation products from 1,2,4-trimethylbenzene, in decreasing order of significance: 3-methyl-3-hexene-2,5-dione, 2,3-dimethyl-2-butenedial, 3-methyl-4-oxo-2-pentenal, and 3-hexene-2,5-dione. Similar to 3-hexene-2,5-dione in the *p*-xylene photooxidation mechanisms, 3-methyl-3-hexene-2,5-dione can partition into the particle phase, and may be photolytically excited to break one bond of the double bond, to make an alkyl bi-radical. Water, a nitrophenol, or one of the carboxylic acids, upon interaction with this alkyl bi-radical, will yield a hydrogen, resulting in an alkyl radical and a hydroxyl or phenoxy radical. The alkyl radical will abstract another hydrogen from another water molecule or nitrophenol molecule to yield 3-methyl-2,5-hexanedione. This process is outlined in Figure 3.7. The subsequent photoisomerization and oxidation of 3-methyl-4-oxo-2-

pentenal can lead to 3-methyl-2,5-furandione. Further reactions of 3-methyl-4-oxo-2-pentenal are analogous to those of 2-methyl-4-oxo-pentenal in the *m*-xylene photooxidation mechanisms (Bierbach *et al.*, 1994). (Refer to Figure 3.6.) Again, the formation of 2,5-furandione from the photooxidation of 1,2,4-trimethylbenzene is presently uncertain, and may arise from the photooxidation of 3-hexene-2,5-dione as shown in Figure 3.8.

Ethylbenzene Photooxidation Mechanisms

The photooxidation mechanisms of ethylbenzene are shown in Figures 9-12. As with the other aromatics, OH can abstract an H-atom from the alkyl group, or it can add to the ring. The abstraction route leads to the formation of acetophenone and eventually benzaldehyde. Since a secondary alkyl radical is more stable than a primary alkyl radical, the abstraction mechanism results in more acetophenone. Figure 3.9 suggests the steps in H abstraction from ethylbenzene. Similarly to toluene-OH adduct reactions, mechanisms for ethylbenzene-OH adduct reactions leading to ethyl-nitrophenols are suggested in Figure 3.10. Since the exact isomer was not identified, Figure 3.10 suggests pathways for photooxidation of ethylbenzene leading to several ethyl-nitro-phenolic compounds. Assuming similar bicyclic oxy radicals form from ethylbenzene-OH adducts as from toluene-OH adducts, the following ring-fragmentation products can be proposed: 2-butenedial, 4-oxo-2-hexenal, 2-ethyl-2-butenedial. The formation of 2-butenedial and 2-ethyl-2-butenedial are outlined in Figures 11 and 12, respectively, as well as the final products to which these dicarbonyls lead (Andino *et al.*, 1996; Hoshino *et al.*, 1978; Bartolotti and Edney, 1995).

m-Ethyltoluene Photooxidation Mechanisms

For the H-abstraction pathway of *m*-ethyltoluene, OH radical attack can occur at the methyl group or the ethyl group. The probable course of H-abstraction from the ethyl group is shown in Figure 3.9. This pathway leads to 3'-methylacetophenone and eventually *m*-tolualdehyde. Similar to the mechanism in Figure 3.1, 3-ethylbenzoic acid results from the H-abstraction on the methyl group to form 3-ethylbenzaldehyde, and subsequent oxidation of the aldehyde to the carboxylic acid. Andino *et al.* (1996) proposed the following ring-fragmentation products from the *m*-ethyltoluene-OH adducts: 4-oxo-2-hexenal, 4-oxo-2-pentenal, 2-methyl-2-butenedial, 2-methyl-4-oxo-2-hexenal, 2-ethyl-2-butenedial, and 2-ethyl-4-oxo-2-pentenal. As illustrated in Figures 3 and 6, 2-methyl-2-butenedial, 4-oxo-2-pentenal, and 2-ethyl-4-oxo-2-pentenal lead to 3-methyl-2,5-furandione, 2,5-furandione, and 3-ethyl-2,5-furandione, respectively. These mechanisms can be extended to predict fates of the remaining dicarbonyl ring-fragmentation products. Figure 3.13 proposes a pathway similar to that in Figure 3.6, leading to 2,5-furandione from 4-oxo-2-hexenal. (4-Oxo-2-hexenal is also formed in the ethylbenzene-OH oxidation.)

p-Ethyltoluene Photooxidation Mechanisms

Hydroxyl reaction resulting in H-abstraction and the products 4'-methylacetophenone and *p*-tolualdehyde is outlined in Figure 3.9. The OH addition pathway is adapted from the treatment of Andino *et al.* (1996) on *p*-xylene. The proposed mechanisms leading to the ring-fragmentation products 2-methyl-2-butenedial, 2-ethyl-2-butenedial, and 3-heptene-2,5-dione are shown in Figures 14, 15, and 16, respectively. These products can further react as depicted in Figures 3, 12, and 8, to form 3-methyl-2,5-furandione, 3-ethyl-2,5-furandione, and 2,5-furandione, which were detected in the *p*-ethyltoluene SOA.

Acknowledgments

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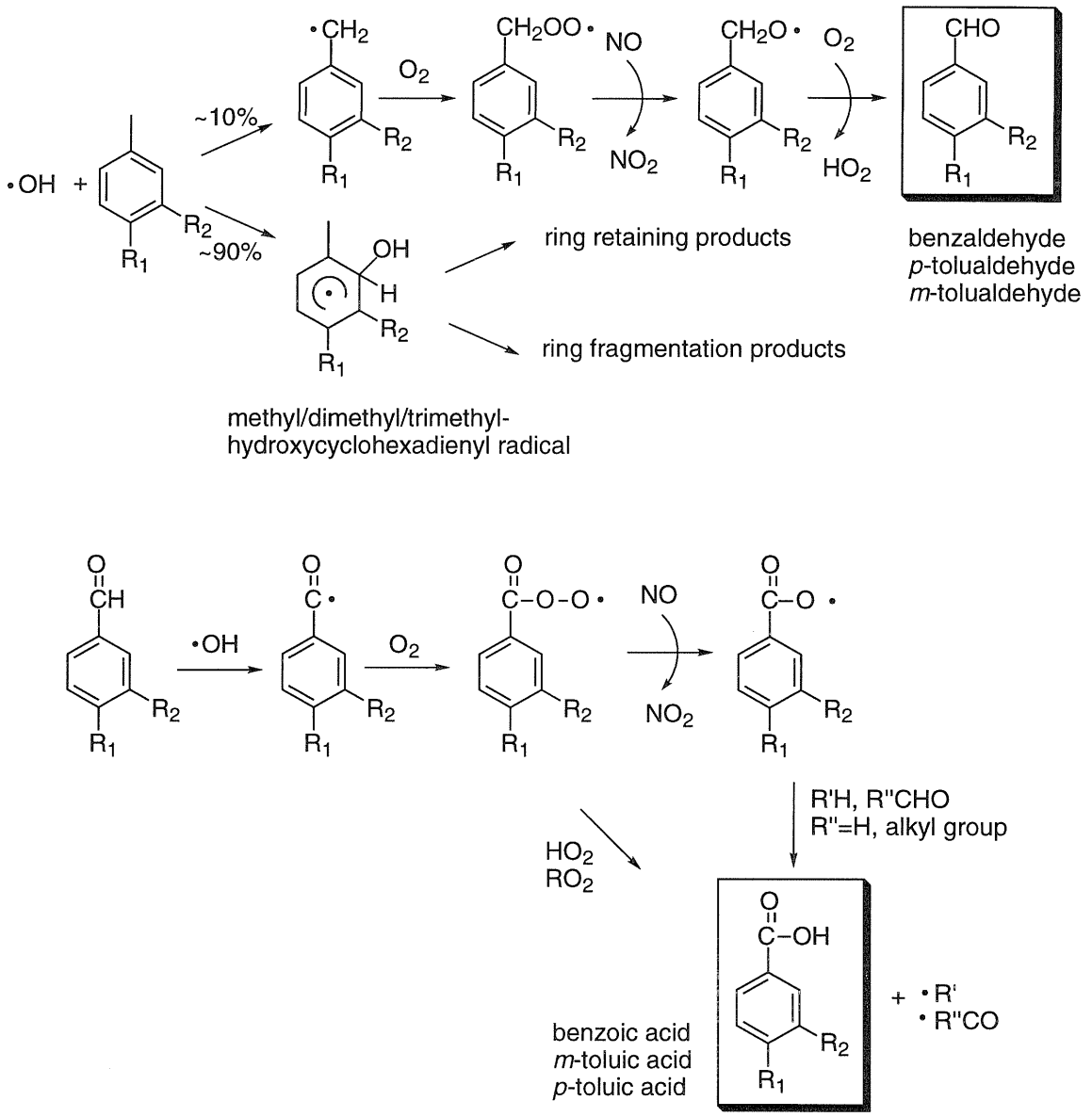


Figure 3.1. Toluene-, *m*-Xylene-, *p*-Xylene-OH initial reaction split and details of abstraction path. R_1, R_2 = H for toluene. R_1=CH_3, R_2=H for *p*-xylene. R_1=H, R_2=CH_3 for *m*-xylene.

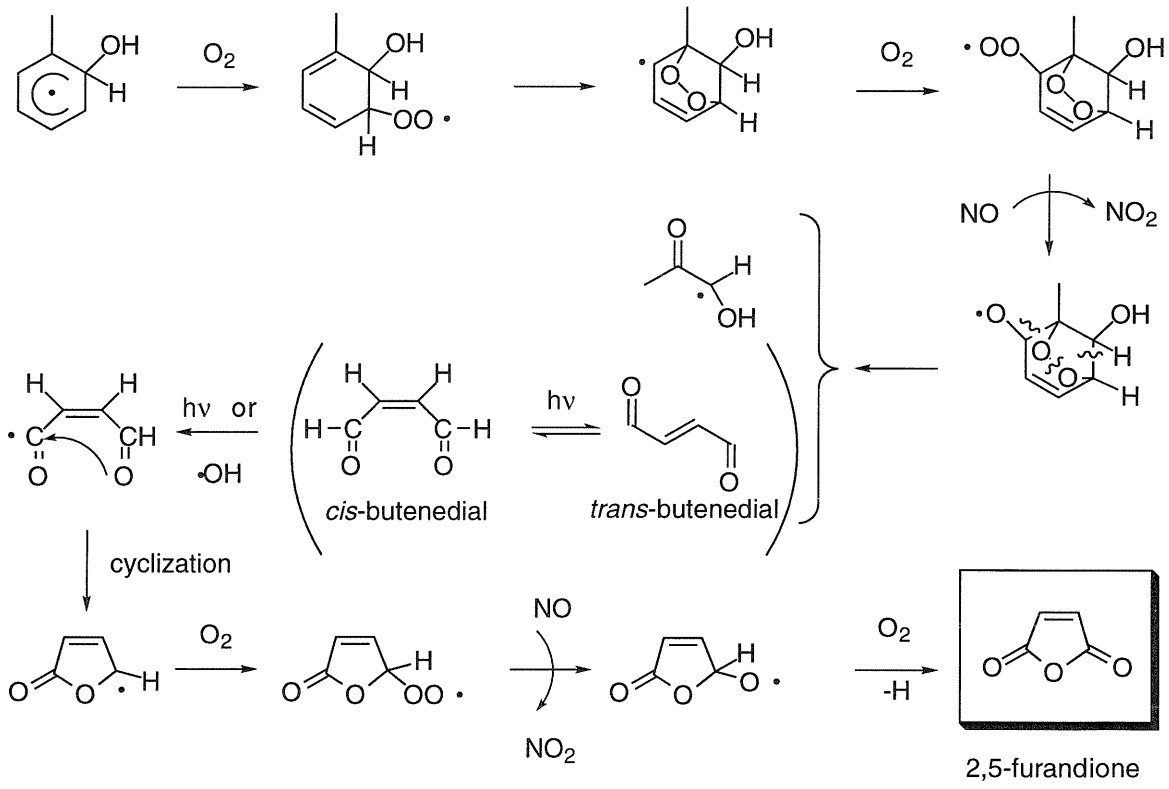


Figure 3.2. Toluene-OH pathway leading to 2,5-furandione (Bierbach *et al.*, 1994).

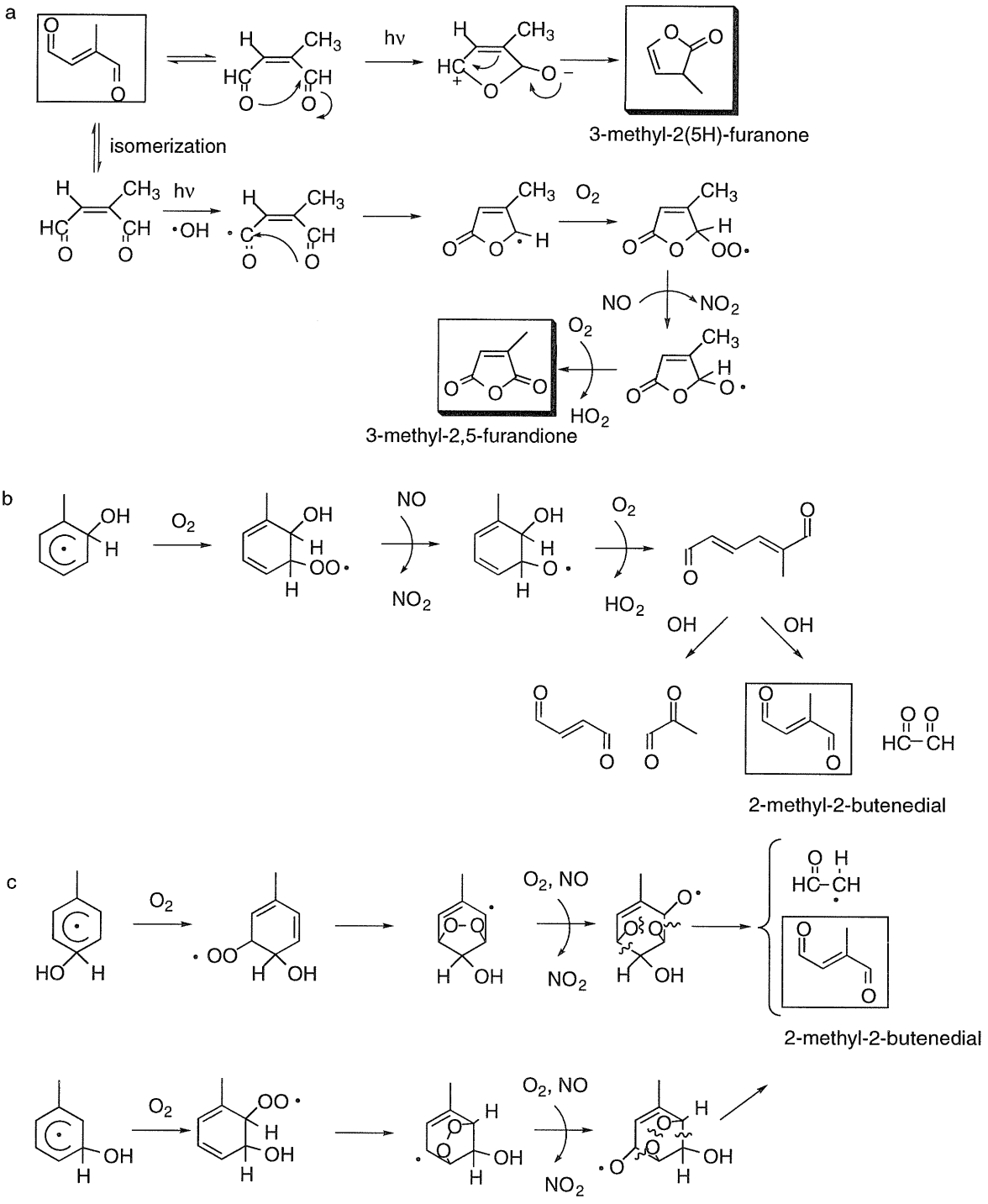


Figure 3.3. Mechanisms of toluene-OH reaction leading to 3-methyl-2,5-furandione and 3-methyl-2(5H)-furanone.

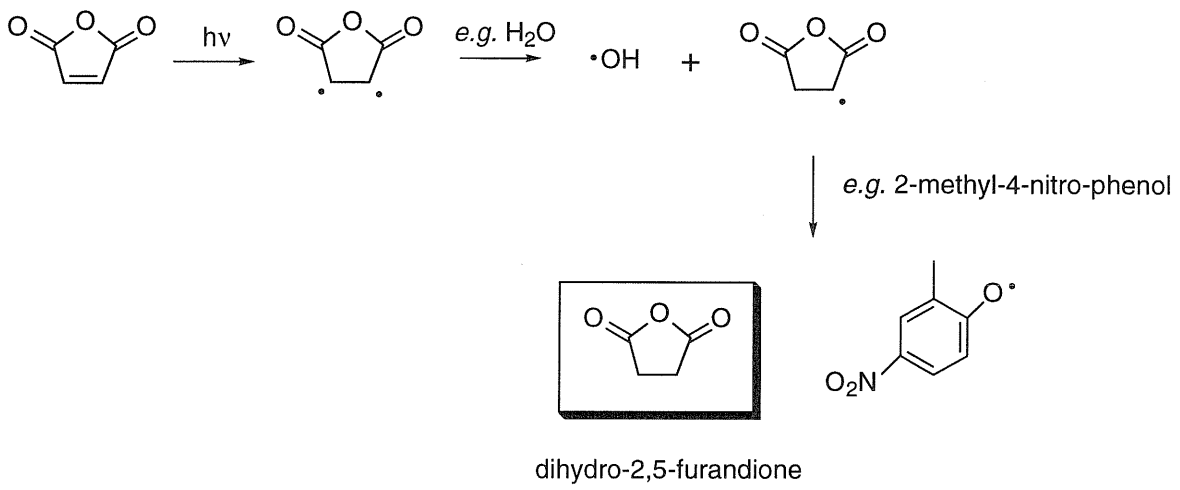


Figure 3.4. Photolytically-induced mechanism from 2,5-furandione to dihydro-2,5-furandione.

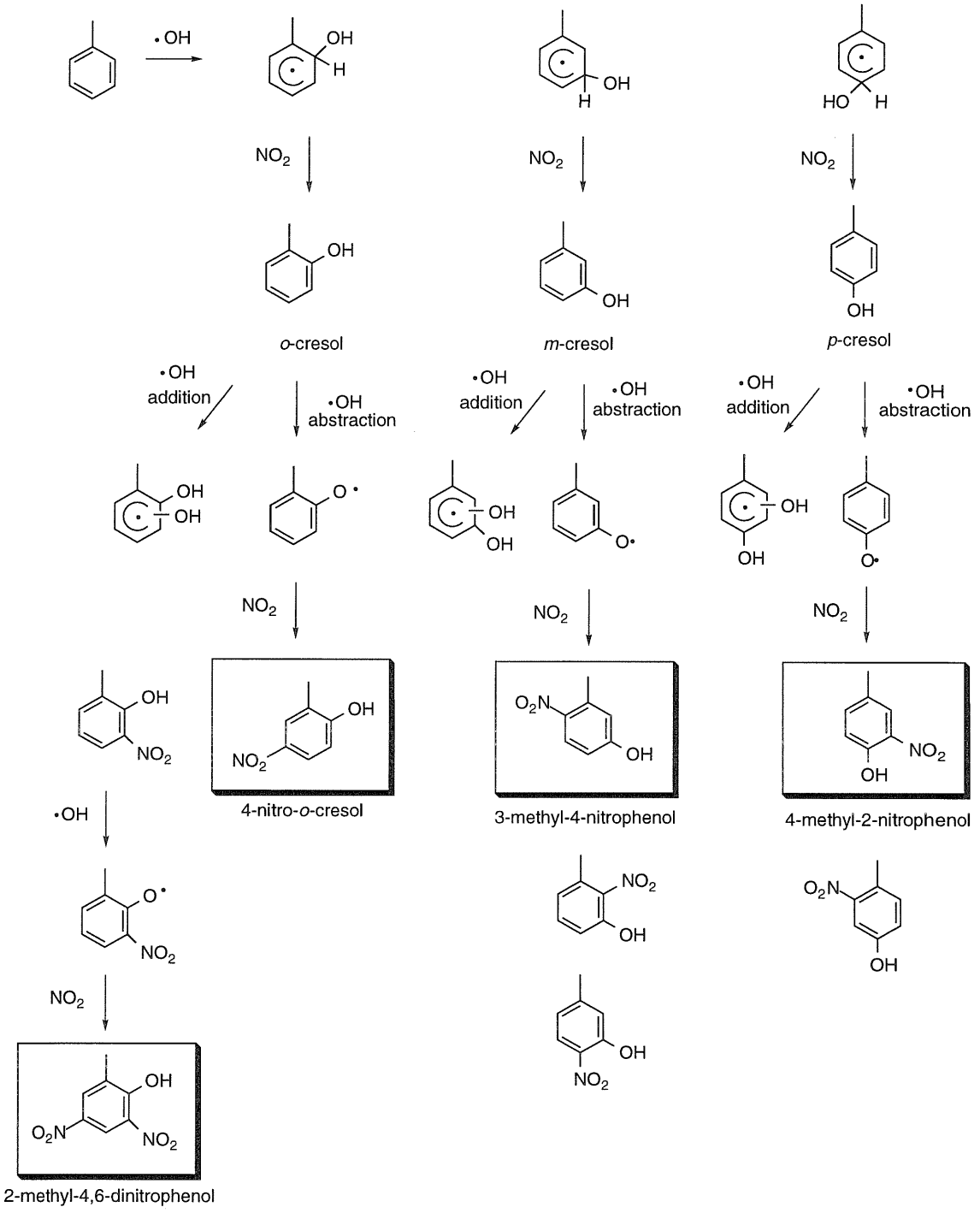


Figure 3.5. Reactions of NO_2 with the methyl-hydroxycyclohexadienyl radical resulting from toluene-OH reaction leading to observed organic aerosol products.

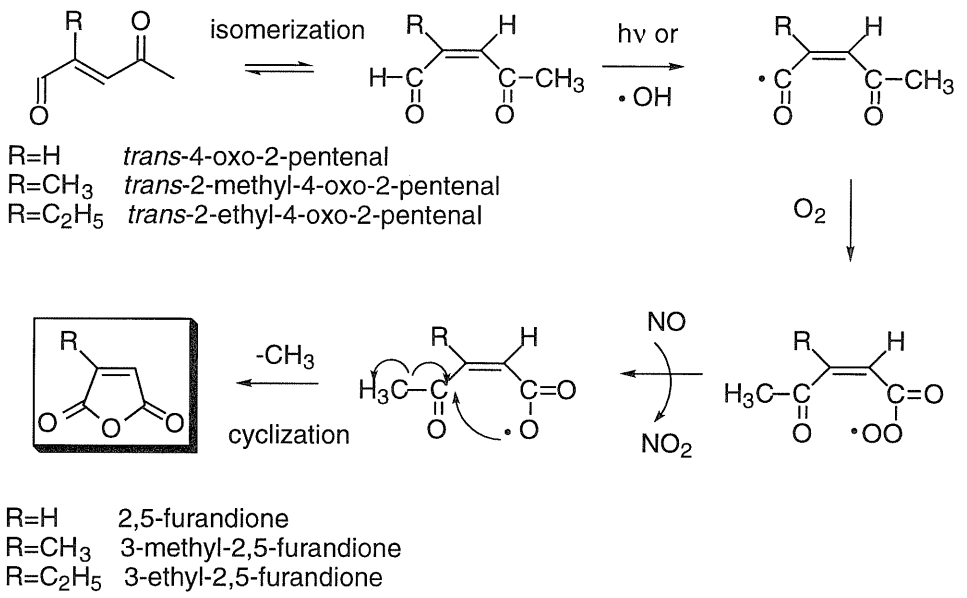


Figure 3.6. Formation of 2,5-furandione from *trans*-4-oxo-2-pentenal, formation of 3-methyl-2,5-furandione from *trans*-2-methyl-4-oxo-2-pentenal (R=CH_3), and formation of 3-ethyl-2,5-furandione from *trans*-2-ethyl-4-oxo-2-pentenal (R=C_2H_5).

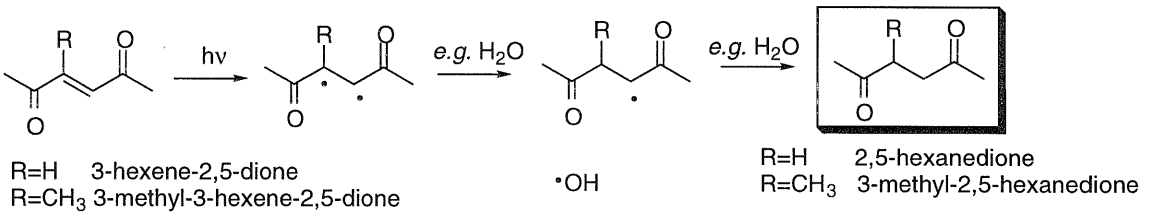


Figure 3.7. Photolytically-induced mechanism from 3-hexene-2,5-dione to 2,5-hexanedione, and from 3-methyl-3-hexene-2,5-dione to 3-methyl-2,5-hexanedione.

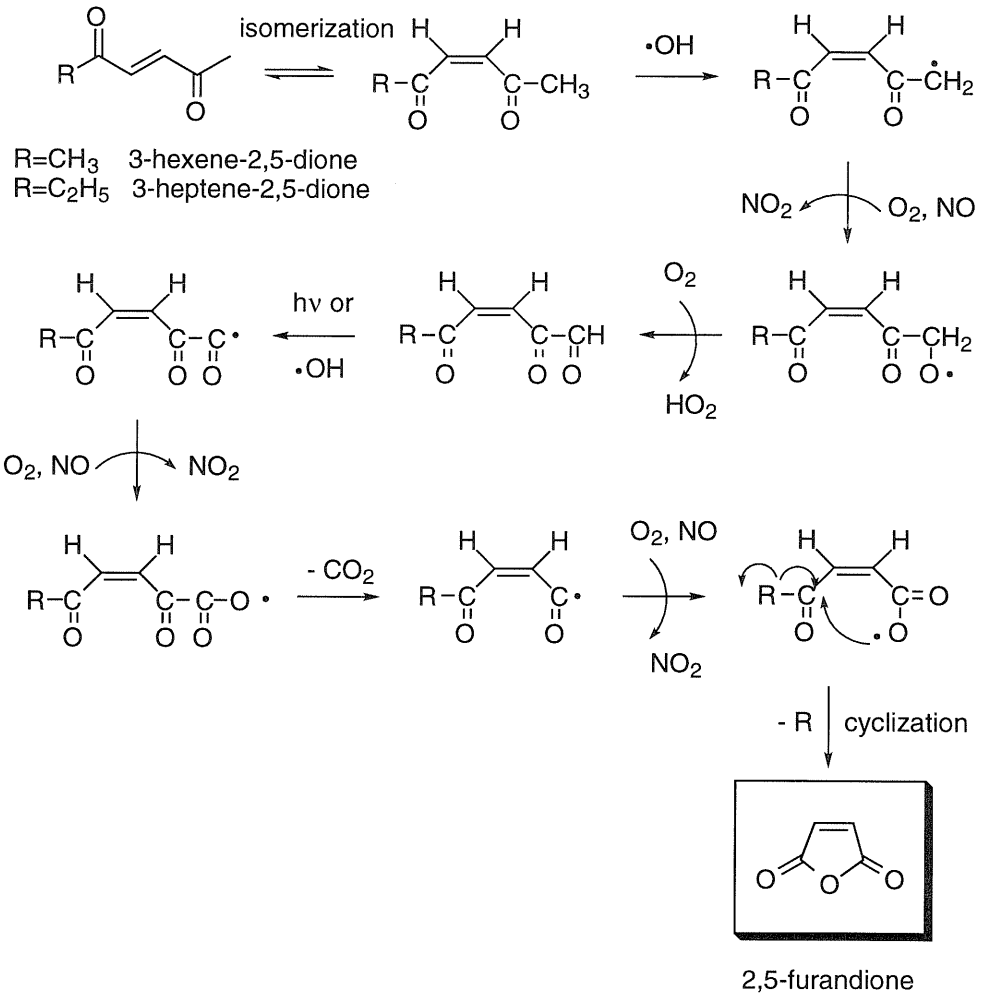


Figure 3.8. Formation of 2,5-furandione from 3-hexene-2,5-dione and from 3-heptene-2,5-dione.

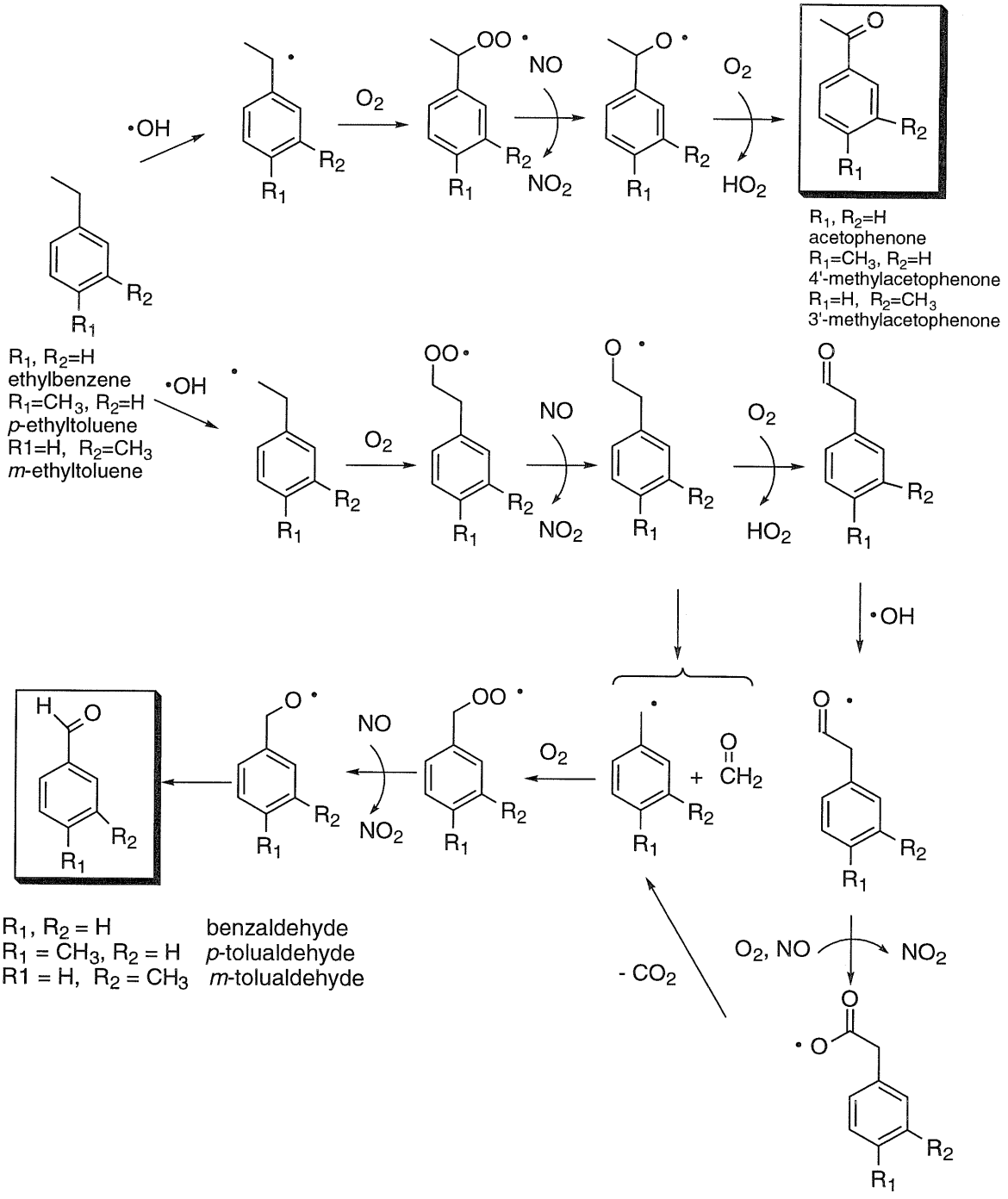


Figure 3.9. Ethylbenzene-OH pathway leading to acetophenone and benzaldehyde. *p*-Ethyltoluene-OH pathway leading to 4'-methylacetophenone and *p*-tolualdehyde. *m*-Ethyltoluene-OH pathway leading to 3'-methylacetophenone and *m*-tolualdehyde.

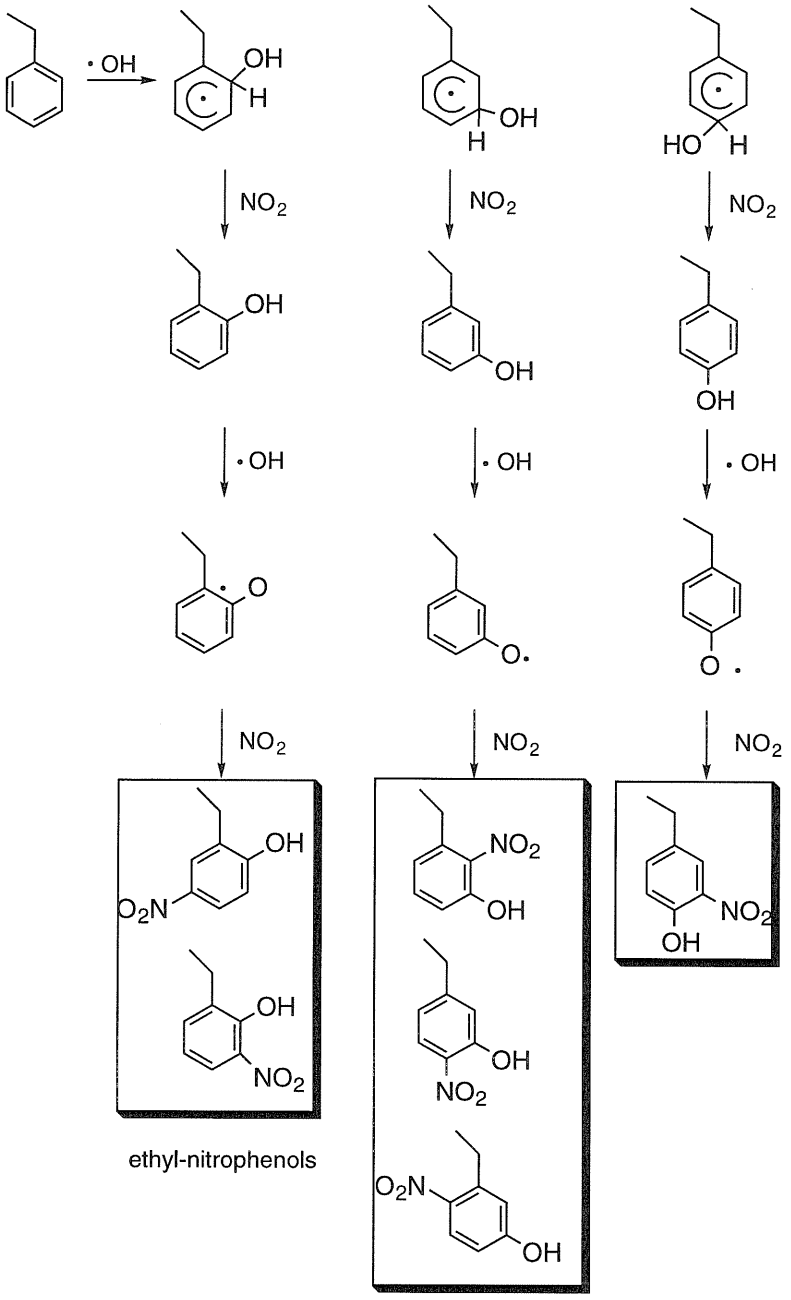


Figure 3.10. Suggested pathways of ethylbenzene-OH adduct leading to ethyl-nitrophenolic compounds.

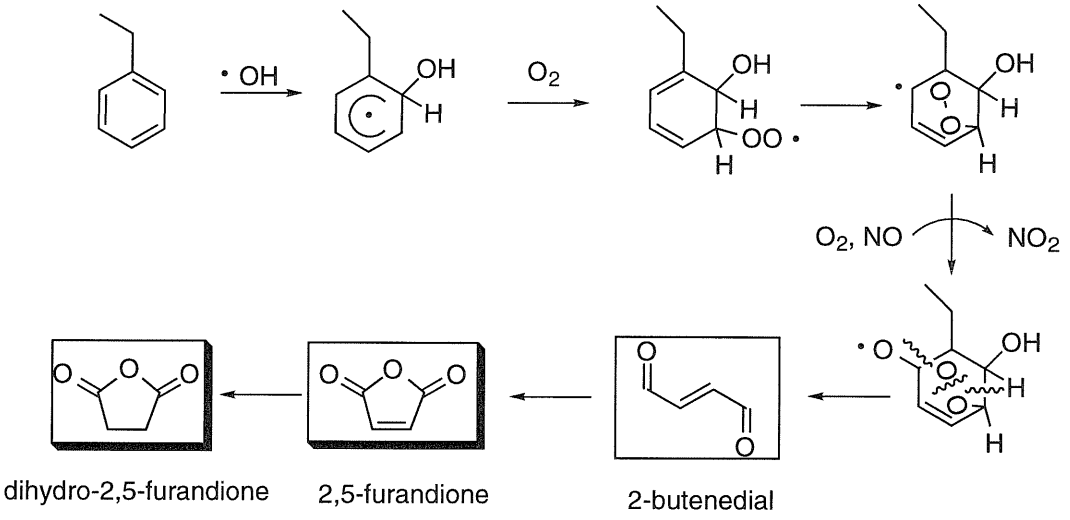


Figure 3.11. Pathway leading to 2-butenedial from ethylbenzene-OH adduct.

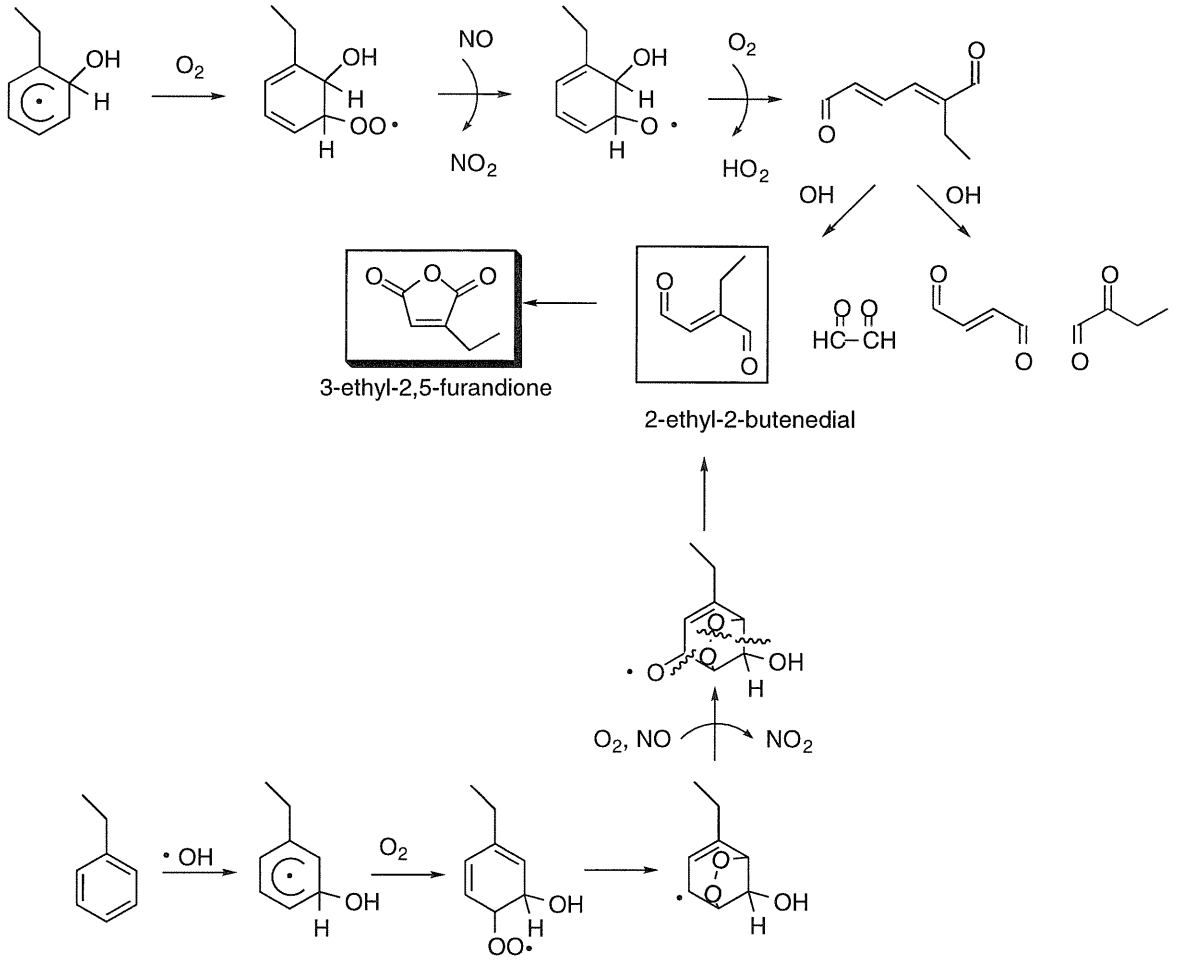


Figure 3.12. Pathway leading to 2-ethyl-2-butenedial from ethylbenzene-OH adduct.

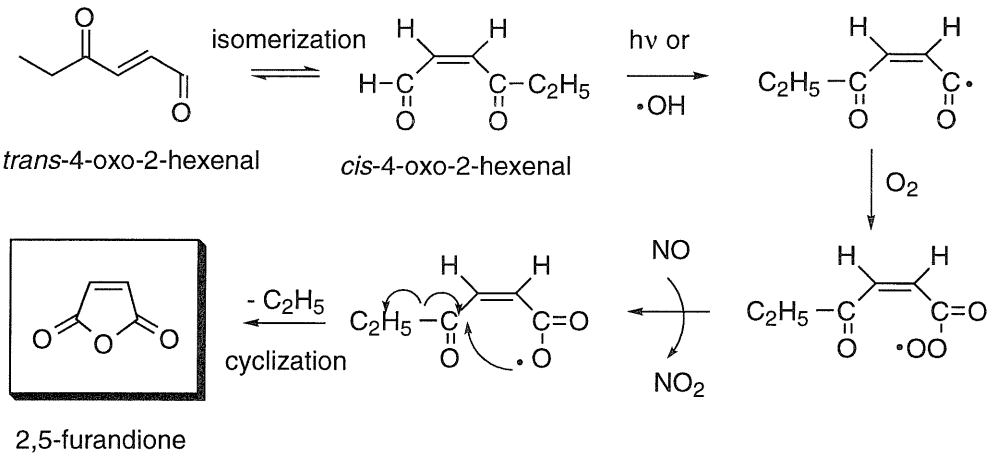


Figure 3.13. Pathway leading to 2,5-furandione from *m*-ethyltoluene photooxidation.

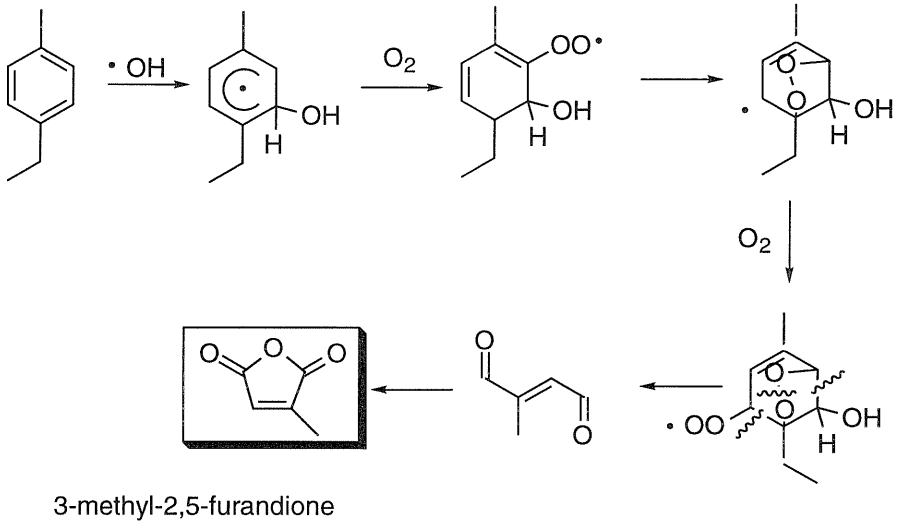
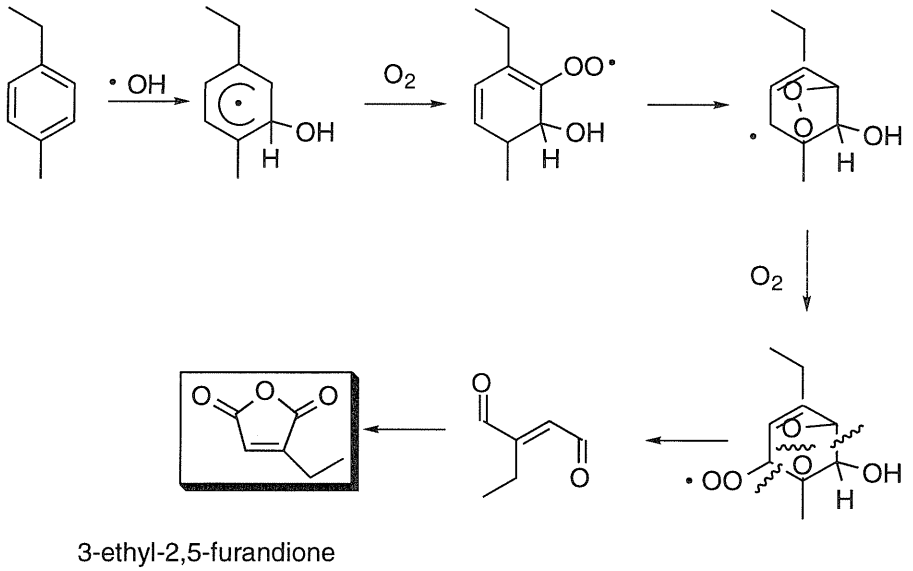


Figure 3.14. Pathway leading to 2-methyl-2-butenedial from *p*-ethyltoluene-OH adduct.



3-ethyl-2,5-furandione

Figure 3.15. *p*-Ethyltoluene-OH adduct fragmentation pathway leading to 2-ethyl-2-butenedial.

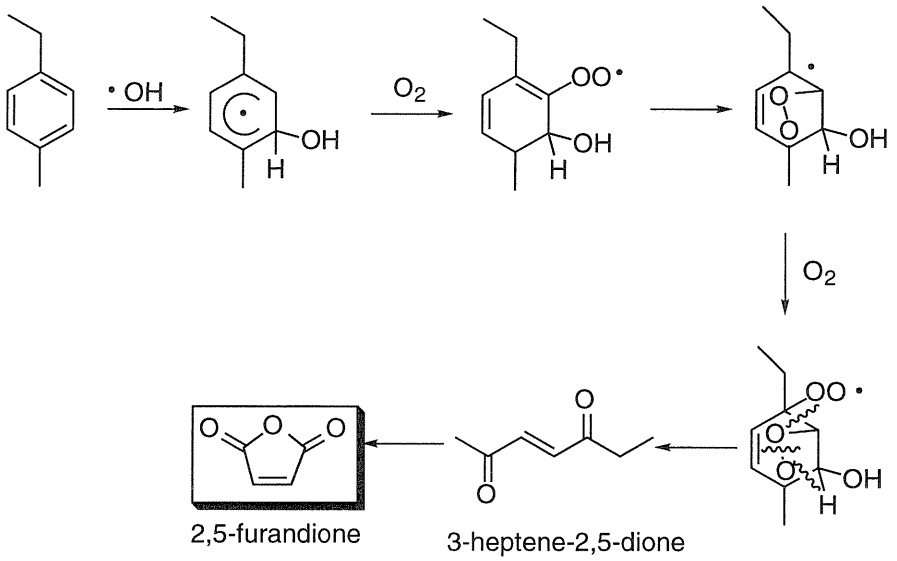


Figure 3.16. *p*-Ethyltoluene-OH adduct fragmentation pathway.

Table 3.1. Initial conditions for 1993 outdoor smog chamber experiments.

aromatic	**[HC]** ppm	**[C_3H_6]** ppm	**initial particles** cm^{-3}	**[NO]** ppm	**[NO_2]** ppm	**HC:NO_x ratio** ppbC/ppb
toluene	4.2	1.5	420	1.0	0.45	23
toluene	6.0	1.6	350	1.0	0.49	31
toluene	2.5	1.1	560	0.61	0.28	23
m-xylene	2.7	-	690	0.63	0.29	26
m-xylene	8.6	1.5	430	1.1	0.55	43
m-xylene	6.5	1.3	270	1.2	0.57	31
p-xylene	4.7	1.3	520	1.2	0.56	24
p-xylene	2.5	1.0	320	0.70	0.31	23
p-xylene	6.3	1.5	420	1.2	0.57	31

Table 3.2. Compounds identified in secondary organic aerosol from aromatic photooxidation. (Numbers given are percentages of the total identified mass for the particular precursor aromatic.)

compound	toluene	*m*-xylene	*p*-xylene	1,2,4-trimethylbenzene	ethylbenzene	*m*-ethyltoluene	*p*-ethyltoluene
2'-hydroxy-5'-methylacetophenone						0.11 ± 0.06	
2,3,5-trimethyl-1,4-benzoquinone [a]				0.04 ± 0.07			
2,4-dimethylbenzaldehyde				0.76 ± 0.82			
2,4-dimethylphenol		0.24 ± 0.27		0.03 ± 0.04			
2,5-dimethyl-1,4-benzoquinone [b]			0.46 ± 0.73				
2,5-dimethylbenzaldehyde				0.46 ± 0.57			
2,5-dimethylphenol			1.9 ± 2.7	1.2 ± 1.0			
2,5-furandione	9.6 ± 1.1	5.2 ± 4.2	1.7 ± 1.3	7.0 ± 1.0	16. ± 2.1	7.4 ± 3.4	4.9 ± 0.60
2,5-heptadione							1.0 ± 1.0
2,5-hexanedione			5.6 ± 3.0			1.6 ± 0.18	1.6 ± 0.89
2,6-dimethyl-1,4-benzoquinone [a]		0.44 ± 0.40					
2,6-dimethyl-4-nitrophenol		3.3 ± 0.86					
2,6-dimethylphenol		+					
2-acetyl-5-methylfuran		4.1 ± 3.0	2.0 ± 0.99	0.26 ± 0.11	0.48 ± 0.42	0.12 ± 0.02	0.42 ± 0.24
2-ethyl-1,4-benzoquinone [a]					1.5 ± 0.42		
2-furaldehyde	0.15 ± 0.02		0.05 ± 0.06				
2-hydroxy-5-nitrobenzaldehyde	1.6 ± 1.2						
2-methyl-1,4-benzoquinone [b]	0.46 ± 0.35						
2-methyl-4,6-dinitrophenol	3.5 ± 4.0	0.39 ± 0.31					
3,4,5-trimethyl-2(3H)-furanone [c]				2.0 ± 2.2			
3,4-dimethylbenzaldehyde				0.83 ± 0.98			
3,4-dimethylbenzoic acid				12. ± 2.2			
3,4-dimethylfurandione		0.41 ± 0.36	0.19 ± 0.27	3.1 ± 1.5	0.12 ± 0.16		
3,4-dimethylphenol							+
3,4/4,5-dimethyl-2(3H)-furanone [c]				0.78 ± 0.25			
3,5-dimethyl-2(3H)-furanone [c]		0.49 ± 0.29					
3,5-dimethyl-2H-pyran-2-one		2.7 ± 2.1					
3-acetyl-2,5-dimethylfuran			0.32 ± 0.34	0.09 ± 0.05		1.1 ± 0.85	

3-ethyl-2(5H)-furanone [d]						0.42 ± 0.25	0.16 ± 0.10
3-ethyl-2,5-furandione [e]					7.4 ± 3.8	24. ± 12.	35. ± 5.0
3-ethyl-5-methyl-2(3H)-furanone [f]						0.07 ± 0.06	
3-ethylbenzaldehyde						1.9 ± 0.81	
3-ethylbenzoic acid						6.6 ± 2.2	
3-hydroxybenzaldehyde	0.04 ± 0.05						
3'-methylacetophenone						12. ± 5.9	
3-methyl-2(5H)-furanone	1.4 ± 0.39	0.89 ± 0.49	1.9 ± 2.1				1.0 ± 0.35
3-methyl-2,5-furandione	26. ± 3.6	61. ± 14.	53. ± 27.	27. ± .0	17. ± 5.5	18. ± 6.4	16. ± 7.2
3-methyl-2,5-hexanedione [g]				9.9 ± 2.0			
3-methyl-4-nitrophenol	6.8 ± 0.80	2.1 ± 1.9					
3-methyl-5-ethyl-2(3H)-furanone [h]						1.3 ± 0.59	
3-methylbenzyl alcohol		0.38 ± 0.66					
3'-nitroacetophenone					1.6 ± 0.56		
3-nitrotoluene	0.18 ± 0.02		0.04 ± 0.05				
4'-hydroxy-3'-nitroacetophenone					1.5 ± 1.5		0.34 ± 0.10
4'-hydroxyacetophenone						0.52 ± 0.27	0.41 ± 0.05
4-ethylbenzaldehyde							4.0 ± 1.6
4-ethylbenzoic acid							4.7 ± 0.64
4-ethylnitrobenzene					1.8 ± 0.53		
4-hydroxy-3-methylbenzaldehyde		0.03 ± 0.06					
4'-methylacetophenone							15. ± 5.1
4-methylphthalic acid				28. ± 5.3			
4-methyl-2-nitrophenol	4.4 ± 1.4		6.0 ± 7.6				4.1 ± 1.2
4-methylbenzyl alcohol			1.8 ± 1.9				
2-methyl-4-nitro-phenol [i]	10. ± 0.12						
5-ethyl-2(3H)-furanone [j]					0.17 ± 0.24	1.4 ± 1.5	
5-ethyl-2-furaldehyde					3.6 ± 2.0	0.29 ± 0.51	
5-methyl-2(3H)-furanone	2.9 ± 1.6	3.1 ± 1.6		0.15 ± 0.13	0.62 ± 0.41	0.56 ± 0.22	0.31 ± 0.27
5-methyl-2-furancarboxaldehyde	1.6 ± 0.23		2.1 ± 2.0	1.8 ± 0.34	2.1 ± 3.0		0.91 ± 0.19
5-methylfurfural		0.84 ± 0.60					
acetophenone					19. ± 7.8	0.19 ± +	+

α-methylbenzene methanol						0.03 ± 0.06	
benzaldehyde	3.0 ± 0.46	1.4 ± 1.4	0.75 ± 0.67	3.8 ± 0.71	7.8 ± 3.7	2.6 ± 1.7	1.8 ± 0.39
benzoic acid	5.4 ± 1.2					2.8 ± 4.9	
benzyl alcohol	0.72 ± 0.46						
dihydro-2,5-furandione	22. ± 0.09		4.2 ± 4.7		2.5 ± 3.5	6.3 ± 5.6	
dihydro-5-methyl-2(3H)-furanone					9.1 ± 4.7	3.0 ± 3.1	
ethyl-nitrophenol [k]					7.0 ± 1.7		
m-cresol	0.15 ± 0.03						
m-tolualdehyde		3.9 ± 3.0				6.31 ± 3.82	
m-toluic acid		9.2 ± 4.6				1.2 ± 1.0	
o-cresol	0.02 ± 0.02						
p-cresol			0.33 ± 0.35				0.29 ± 0.02
p-tolualdehyde			14. ± 16.				7.1 ± 2.6
p-toluic acid			3.3 ± 4.0				0.86 ± 0.38
phenol	0.09 ± 0.01				0.19 ± +	0.04 ± 0.01	0.02 ± 0.01
sec-phenethyl alcohol					1.3 ± 0.24		
terephthaldicarboxaldehyde							0.33 ± 0.08

[a]Organic tentatively identified from its mass spectra. Contribution estimated using response of 1,4-benzoquinone.

[b]Organic identified by match in Wiley mass spectral library. Contribution estimated using response of 1,4-benzoquinone.

[c]Organic tentatively identified from its mass spectra. Contribution estimated using response of 2,2-dimethyl-3(2H)-furanone.

[d]Organic identified by match in Wiley mass spectral library. This organic could also be 5-ethyl-2(3H)-furanone. Contribution estimated using response of 5-methyl-2(5H)-furanone.

[e]Organic identified by match in Wiley mass spectral library. Contribution estimated using response of 3-methyl-2,5-furandione.

[f]Organic tentatively identified from its mass spectra. This organic could also be 5-ethyl-3-methyl-2(3H)-furanone. Contribution estimated using 3-methyl-2(5H)-furanone.

[g]Organic tentatively identified from its mass spectra. Contribution estimated using 2,5-hexanedione.

[h]Organic tentatively identified from its mass spectra. This organic could also be 3-ethyl-5-methyl-2(3H)-furanone. Contribution estimated using 5-methyl-2(5H)-furanone.

[i]Organic matched reference in NIST mass spectral library. Contribution estimated using 5-methyl-2-nitrophenol.

[j]Organic identified by match in Wiley mass spectral library. Contribution estimated using 5-methyl-2(3H)-furanone.

[k]Organic identified by match in Wiley library. Any isomer could be possible. Contribution estimated using 2,6-dimethyl-4-nitrophenol.

Molecular Speciation of Secondary Organic Aerosol from Photooxidation of the Higher Alkenes: 1-Octene and 1-Decene

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Abstract

Outdoor smog chamber photooxidations to determine the molecular composition of secondary organic aerosol (SOA) from 1-octene and 1-decene in sunlight-irradiated hydrocarbon-NO_x mixtures are reported. The observed products are consistent with the current understanding of alkene reactions with OH and O_3. Gas-phase mechanisms leading to the observed products are outlined. Heptanal, heptanoic acid, and dihydro-5-propyl-2(3H)-furanone were the dominant organics identified in 1-octene aerosol. The corresponding species in 1-decene aerosol were nonanal, nonanoic acid, and dihydro-5-pentyl-2(3H)-furanone. Measured aerosol yields from 1-octene and 1-decene experiments are also reported, and are found to correlate with organic mass concentration according to semi-volatile gas/particle partitioning theory. A new organic aerosol extraction procedure utilizing supercritical CO_2 extraction is outlined.

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Introduction

Alkenes constitute a significant class of volatile organic compounds present in urban atmospheres (Lurmann and Main, 1992). Reactions of alkenes with ozone (O_3), hydroxyl radicals (OH), and nitrate radicals (NO_3) are relevant to ozone formation. For alkenes with carbon numbers greater than about five, the reaction products of the alkenes with ozone and other radicals may lead to secondary organic aerosol (SOA) formation (Grosjean and Seinfeld, 1989). The atmospheric chemistry of the lower molecular weight alkenes has been extensively studied, but that of longer-chain alkenes has only recently received attention (Atkinson, 1994; Grosjean *et al.*, 1996ab; Grosjean and Grosjean, 1996; Kwok *et al.*, 1996a; Paulson and Seinfeld, 1992). The potential of long-chain alkenes to serve as aerosol precursors has been previously investigated, but few studies have systematically addressed the identification of the products comprising the secondary aerosol (Grosjean *et al.*, 1994; Wang *et al.*, 1992). By determining the composition of secondary organic aerosol from alkenes, gas-phase mechanisms leading to these products can be evaluated, thereby extending our understanding of the role alkenes play in atmospheric chemistry.

In this study, the photooxidation of 1-octene and 1-decene in the presence of nitrogen oxides was investigated via outdoor smog chamber studies, with particular emphasis on determining the molecular composition of the resulting secondary organic aerosol. 1-Octene and 1-decene were chosen because of their presence in urban atmospheres and their known aerosol-forming potential (Grosjean and Seinfeld, 1989; Wang *et al.*, 1992; Grosjean *et al.*, 1994).

Experimental Description

Secondary Organic Aerosol Sample Generation. The outdoor smog chamber facility has been described previously (Forstner, 1996; Wang *et al.*, 1992). An 8 m^3 outdoor Teflon chamber was used for NO_X-air photooxidation of the alkenes. As the goal of these experiments was to generate sufficient secondary aerosol for subsequent analysis, initial hydrocarbon mixing ratios ranged from 2 to 8 ppm. Initial hydrocarbon-NO_X ratios were at least 25 ppmC/ppm, a level that has been previously found to be optimal for secondary organic aerosol formation (Zhang *et al.*, 1992). Initial particles were also injected into the smog chamber at concentrations near 1000 cm^{-3}. Ammonium sulfate seed aerosol, used to encourage condensation of the secondary gas-phase products, had an initial particle size distribution ranging from 10 nm to about 200 nm diameter, with the distribution centered at 65 nm. Table 4.1 lists the initial conditions of the 1-octene and 1-decene experiments performed.

Sample Collection. Aerosol size distribution measurements were performed with a differential mobility analyzer (DMA, TSI Model 3071) and a condensation nuclei counter (CNC, TSI Model 3760). The DMA and CNC were operated as a scanning electrical mobility spectrometer (SEMS) (Wang and Flagan, 1990) and generated particle size distributions every minute with a size range of about 10 nm to 200 nm. Once significant secondary aerosol had formed, as evidenced by growth of the seed particles, aerosol was collected. Sampling typically began 4 to 6 h into an experiment. The smog chamber was deflated through filter samplers, each operating at 10 L min^{-1}. Quartz fiber filters 47 mm in diameter from Pallflex (Putnam, CT) were used. Prior to usage, the filters were baked at 750 °C for at least 2 h. Blank, baked filters were extracted and found to have no background contamination. The filters were stored in glass jars with Teflon-lined lids at sub-zero temperatures immediately after collection. The storage jars were prepared prior to use by rinsing in distilled water, then twice with HPLC-grade methanol, and finally in

HPLC-grade methylene chloride. The open ends of the jars were covered with foil and the jars were baked at 550 °C for at least 4 h. The filter samplers and the Teflon-lined lids of the jars were similarly cleaned by sonication in distilled water, then in HPLC-grade methanol, and finally in HPLC-grade hexane. The above protocol is similar to that employed by Hildemann *et al.* (1991).

Sample Extraction. A new extraction protocol using supercritical CO_2 has been developed for the quantitative analysis of secondary organic aerosol samples from smog chamber experiments and is outlined in the following Appendix. The extraction method was optimized by recovery studies of filters impregnated with 5 to 50 µl of an organic standard. The compounds in the organic standard are listed in the Appendix. These compounds were chosen as they have either been previously identified as gas-phase oxidation products (Paulson and Seinfeld, 1992; Atkinson, 1994) or they have relevant functional groups, for example, nitrates and hydroperoxides. Numerous extractions of the recovery standard were performed and no conversion of any of the species in the standard were observed. The SFE-GC/MS system does not appear to induce any reaction of the analytes. The optimal method was found to be extraction using supercritical CO_2, modified with a 10% solution of acetic acid in methanol. The Suprex PrepMaster (Pittsburgh, PA) extraction unit and modifier pump were used. The filters were allowed to equilibrate in CO_2 at 150 °C and 420 atm for 10 min. Then the filters were extracted for 30 min with CO_2 flowing at approximately 1 ml min^{-1}. Modifier was added at a rate of 2% of the CO_2 flow rate. Analytes and CO_2 passed directly through a heated transfer line to the gas chromatograph (GC). The GC column was cryo-cooled to -30 °C, trapping the analytes in the first few meters of the column while allowing the CO_2 to vent. Once the extraction was complete, the GC stepped through its temperature program.

GC/MS Analysis. A Hewlett Packard 5890 Series II gas chromatograph and a Hewlett Packard 5989A mass spectrometer engine were used. After high resolution

chromatography using an HP-1701 60m fused silica column (14% cyanopropyl-phenyl methyl-polysiloxane) with a film thickness of 0.25 μm and inner diameter of 0.25 mm, the MS analyses were performed by electron impact ionization. The Hewlett Packard ChemStation software (HP G1034C), in conjunction with the Wiley library of organic spectra, was employed to initially identify organic compounds in the samples. Except for dihydro-5-propyl-2(3H)-furanone and dihydro-5-pentyl-2(3H)-furanone, the species identified in the SOA were later confirmed by matching retention times with authentic standards and then quantified. Quantification of the two aforementioned compounds was accomplished using the response of 5-ethyl-2(3H)-furanone. All standards were purchased from Aldrich Chemical Co. (St. Louis, MO) and were used without further purification.

Results

Measured Aerosol Yield. The aerosol forming potential of 1-octene and 1-decene has been previously studied. Wang *et al.* (1992) reported an average aerosol yield of 4.2% from 1-octene, and Grosjean *et al.* (1994) demonstrated the aerosol-forming potential of 1-decene. Aerosol yield is defined in the present study as the ratio of aerosol volume formed to the amount of parent hydrocarbon reacted. The aerosol size distribution data were corrected for wall losses and then integrated to determine the secondary aerosol volume concentration (*V(t)*), and converted to a mass basis assuming an aerosol density of 1.0 g cm^{-3}. Tables 4.2 and 4.3 list the species, and their densities, identified in secondary organic aerosol from 1-octene and 1-decene. A density of 1.0 g cm^{-3} is seen to be a reasonable approximation. The time-dependent aerosol yields are shown in Figure 4.1 as a function of organic mass concentration, according to the expression developed by Odum *et al.* (1996):

$$Y(t) = M_o(t) \sum_i \frac{\alpha_i K^i_{om}}{1 + K^i_{om} M_o(t)} \qquad (1)$$

where $Y(t)$ is aerosol yield ($\mu g\ m^{-3}/\mu g\ m^{-3}$), $M_O(t)$ is the organic aerosol concentration ($\mu g\ m^{-3}$), α_i is a proportionality constant relating the total amount of compound i in the gas-phase to the total amount of hydrocarbon reacted, and K^i_{om} is the gas/particle partitioning coefficient. This expression incorporates the semi-volatile gas/particle partitioning absorption model of Pankow (1994ab) into the definition of yield. Each measured aerosol yield has an uncertainty associated with it. This error arises primarily from uncertainty in the hydrocarbon measurements, which themselves result from the inconsistency of the gas chromatograph response. The measured aerosol volume is virtually entirely secondary organic product, that is $V(t) >> V_O$. Since the relative humidity of the smog chamber was typically 30% or less at temperatures around 303K, water is not likely to be present in the aerosol phase, and the initial volume of seed aerosol is on the order of 0.01% to 1% of the final aerosol volume. The aerosol yields in Figure 4.1 are taken from approximately the first half of each experiment before the size distribution of the aerosol grew beyond the range of the instrument, and the data are consequently clustered at organic mass concentrations less than 10 $\mu g\ m^{-3}$. For clarity, some experiments were omitted from Figure 4.1 although the remaining data is consistent with the results shown. Extrapolation of the results in Figure 4.1 indicate that 1-octene and 1-decene may form secondary organic aerosol upwards of several percent of the amount of alkene reacted, for organic mass concentrations greater than 100 $\mu g\ m^{-3}$, which is consistent with the results of Wang *et al.* (1992).

Composition of Secondary Organic Aerosol. The fraction of 1-octene secondary organic aerosol that was identified was 37% by mass for the experiment on 93-9-26, 42% by mass for 93-8-22, and nearly 50% by mass for 93-8-28. The fraction of 1-decene secondary aerosol that was identified was 37% by mass for the experiment on 93-9-3, 43% by mass for 93-9-1, and 45% by mass for 93-8-30 and for 93-10-25. These estimates were obtained by comparing the identified peak areas in a given chromatogram to

all peak areas in the chromatogram, and assuming an average MS response to convert peak areas to a mass basis. The unidentified fraction consists of a few peaks that were not identifiable with the Wiley library, together with the unresolved mixture that emerged late in the gas chromatograms. The intent of this study was to identify species in the secondary organic aerosol from the photooxidation of 1-octene and 1-decene, and not perform a total carbon balance on the gas and particle phases. Only the portion of the particle-phase carbon which elutes from the GC is considered.

1-Octene. The species identified in the secondary aerosol resulting from the photooxidation of 1-octene in three smog chamber experiments are shown in Table 4.2. The distribution of the products, expressed as a fraction of the total identifiable mass, was determined utilizing standards to calibrate the GC/MS. The identified fraction of the secondary organic aerosol is primarily composed of heptanal, heptanoic acid, and dihydro-5-propyl-2(3H)-furanone. Hexanal, dihydro-5-methyl-2(3H)-furanone, dihydro-5-ethyl-2(3H)-furanone, 1-hexanol, octanal, dihydro-2(3H)-furanone, 1-nitrohexane, hexanoic acid, and octanoic acid appeared in lesser amounts. As stated previously, these species were confirmed by matching retention times and mass spectra with authentic standards. The distribution of heptanal, heptanoic acid, and dihydro-5-propyl-2(3H)-furanone is consistent over the three experiments considered.

1-Decene. The species identified in the secondary organic aerosol resulting from the photooxidation of 1-decene with nitrogen oxides are shown in Table 4.3. The secondary organic aerosol is composed largely of nonanal, nonanoic acid, and dihydro-5-pentyl-2(3H)-furanone. To a lesser extent, octanal, decanal, octanoic acid, decanoic acid, hexanal, 2-heptanone, heptanal, 1,2-epoxyoctane, 1-octanol, and dihydro-5-ethyl-2(3H)-furanone were identified. The distribution of nonanal, nonanoic acid, and dihydro-5-pentyl-2(3H)-furanone is consistent for the 1-decene experiments on 93-8-30, 93-9-1, and 93-9-3, but is significantly different for 93-10-25. There is a shift from approximately

25% nonanoic acid in the earlier experiments to 7.3%, and a corresponding shift from 14% dihydro-5-pentyl-2(3H)-furanone to 44.3% for the experiment on 93-10-25. A possible explanation is that the average temperatures during the earlier experiments were near 30 °C while the average temperature on 93-10-25 was 24 °C. At lower temperatures more dihydro-5-pentyl-2(3H)-furanone may partition into the particle phase, thereby altering the distribution. The measurement from 93-10-25 is authentic, and further study is necessary to explain the observation.

Estimated Relative Importance of Different Oxidants

A comparison of the pseudo-first order rate constants, $k_{OH}[OH]$, $k_{O3}[O3]$, $k_{NO3}[NO3]$, and $k_{O(^3P)}[O(^3P)]$, in the smog chamber experiments allows identification of the important paths in the photooxidation of 1-octene and 1-decene. The rate constants (k_{OH}, k_{O3}, k_{NO3}, and $k_{O(^3P)}$) for 1-octene and 1-decene are given in Table 4.4. The SAPRC generalized organic/NO_X photooxidation mechanism developed by Carter (1990) was employed to estimate time-dependent concentrations of OH, NO_3, O_3, and $O(^3P)$ for the experiments listed in Table 4.1. Although the SAPRC mechanism does not contain an explicit mechanism for either 1-octene or 1-decene, it includes a generalized mechanism for higher alkenes (>C_2H_4) that accounts for reaction with OH, O_3, NO_3, and $O(^3P)$. The mechanism has been evaluated against approximately 100 alkene experiments carried out in environmental chambers, and for single alkene-NO_X simulations, the model reasonably predicts O_3 maxima with an estimated uncertainty of ±22% and NO oxidation rates with an estimated uncertainty of ±24% (Carter and Lurmann, 1991). The simulations were performed with the rate constants for 1-octene and 1-decene, the generalized alkene mechanism, the inorganic NO_X-air reactions, the reactions of RO_2 and formaldehyde, and wall reactions, as suggested by Carter (1990). The simulations are sufficient to describe qualitatively the relative importance of 1-octene/1-decene reactions with OH, O_3, NO_3, and $O(^3P)$ in these smog chamber studies.

In Figure 4.2, pseudo-first order rate constants are shown as a function of time during the 1-octene experiment conducted on 22 August 1993. For the first 100 min, the OH reaction dominates the chemistry, accounting for 20% of the 1-octene decay. At 100 min, reaction with O_3 surpasses that of OH; increase in $k_{O3}[O_3]$ coincides with the rapid decay of 1-octene after 100 min. Figure 4.3 shows the pseudo-first order rate constants as a function of time for the 1-decene experiment on 30 August 1993. Similar to the 1-octene experiments, the rapid 1-decene decay 100 min into the experiment coincides with the rise in $k_{O3}[O_3]$. Although the initial 1-decene decay is largely a result of OH, in contrast to 1-octene, the initial reaction with $O(^3P)$ is predicted to be faster than with O_3, and hence $O(^3P)$ chemistry should be considered as well.

Gas-Phase Chemical Mechanisms Leading to Observed Aerosol Products

Aldehyde Formation. Products identified in the aerosol phase are highlighted in Figures 4.4-4.12. In these experiments, the formation of heptanal from 1-octene, and correspondingly nonanal from 1-decene, arise from the reaction of the alkene with O_3 and OH. Heptanal and nonanal result from the addition of ozone across the double bond in 1-octene and 1-decene, respectively. The current understanding is that ozone forms a 1,2,3-trioxolane adduct which then decomposes into two excited Criegee biradicals and two aldehydes: heptanal/nonanal and formaldehyde (Atkinson, 1994; Grosjean *et al.*, 1996b). The excited biradicals, denoted as $[]^{\ddagger}$, may thermally stabilize or decompose to form other products, of which one path leads to the formation of heptanal/nonanal (see Figure 4.4.).

Figure 4.5 demonstrates the formation of heptanal and nonanal from OH attack on the two alkenes. OH may add to either end of the double bond, but addition to the terminal carbon results in a more stable radical (Streitwieser and Heathcock, 1976). The β-hydroxyalkyl radical rapidly adds O_2. After conversion of NO to NO_2, the resulting β-hydroxyalkoxy radical can then decompose to heptanal/nonanal. Figure 4.5 also

contains a suggested pathway to hexanal/octanal from the initial OH attack. Grosjean *et al.* (1996b) detected hexanal and octanal from reaction of 1-octene and 1-decene with O_3. They suggest an alternative mechanism originating from the initial O_3 attack on 1-octene/1-decene to form hexanal/octanal.

Carboxylic Acid Formation. In addition to heptanal and nonanal, the secondary organic aerosol of 1-octene and 1-decene is composed largely of heptanoic acid and nonanoic acid, respectively. One possible route to carboxylic acid is from oxidation of the aldehyde. Figure 4.6 suggests a possible course involving H-abstraction by OH from the aldehyde, and subsequent addition of O_2 to form a peroxy radical. This radical can react with NO to form NO_2 and an alkoxy radical. The alkoxy radical can further react with another alkene or another aldehyde such as heptanal/nonanal or formaldehyde to abstract an H-atom, resulting in the formation of heptanoic acid/nonanoic acid. Other routes leading to the production of heptanoic acid and nonanoic acid are also possible. The peroxy radical in Figure 4.6, $RC(O)OO\bullet$, may react with $HO_2\bullet$ or $RO_2\bullet$ to yield heptanoic or nonanoic acid. Studies of peroxymethylene and water provide evidence for the formation of formic acid via the following sequence (Hatakeyama *et al.*, 1981):

$$CH_2OO + H_2O \longrightarrow [CH_2OO \cdot H_2O] \longrightarrow HCOOH + H_2O$$

It is possible that the formation of C_7 and C_9 carboxylic acids occurs from isomerization of the thermally stable biradical with the process being similarly facilitated by water. A possible course for the isomerization is shown in Figure 4.4. Another mechanism by which heptanoic acid and nonanoic acid are formed is the immediate isomerization of the excited biradical, which is also outlined in Figure 4.4 (Atkinson, 1994; Atkinson and Lloyd, 1984).

Detectable amounts of octanal and octanoic acid were identified in the 1-octene aerosol samples. Similarly, small quantities of decanal and decanoic acid were identified in the 1-decene aerosol samples. Paulson and Seinfeld (1992) investigated the gas-phase

chemistry of 1-octene with O_3, OH, and $O(^3P)$. They found that octanal, 1,2-epoxyoctane, and 2-octanone arose from the addition of $O(^3P)$. A generalized mechanism of $O(^3P)$ adding to an alkene and producing the aldehyde is shown in Figure 4.7. Noting the low yields of octanal in the mixed oxidant experiments of Paulson and Seinfeld (1992) in addition to consideration of Figure 4.2, it is reasonable that very little octanal and decanal were detected in the aerosol. As outlined in Figure 4.6, the production of the corresponding carboxylic acids possibly results from the atmospheric oxidation of the aldehydes.

Lactone Formation. The remaining significant portion of the aerosol was identified as dihydro-5-propyl-2(3H)-furanone for 1-octene and dihydro-5-pentyl-2(3H)-furanone for 1-decene. Wang *et al.* (1992) suggested two potential mechanisms for the formation of dihydro-5-propyl-2(3H)-furanone from heptanal and from the C_7-Criegee biradical. These two mechanisms are shown in Figure 4.8. Heptanal may lead to dihydro-5-propyl-2(3H)-furanone from an initial OH radical attack with subsequent oxygen addition. Internal cyclization of the α-carbonyl alkoxy radical results in the lactone. Wang *et al.* (1992) also proposed the direct rearrangement of the C_7-Criegee biradical to form the α-carbonyl alkoxy radical and then dihydro-5-propyl-2(3H)-furanone.

It is generally known that these lactones are readily formed from γ-hydroxycarboxylic acids (Streitwieser and Heathcock, 1976). The conversion of the γ-hydroxycarboxylic acid to its lactone is particularly facile in the presence of a small amount of acid, and the equilibrium shifts to the lactone when there are numerous alkyl substituents on the lactone. The detailed mechanism of lactone formation from γ-hydroxycarboxylic acids has been extensively investigated and is outlined in Figure 4.9 (Streitwieser and Heathcock, 1976). If γ-hydroxycarboxylic acids form from the photooxidation of alkenes, the origin of the lactones can arise from four sources. Firstly, the conversion from the γ-hydroxycarboxylic acid to the lactone may occur in the particle phase. The presence of heptanoic acid or

nonanoic acid in the particle phase would be sufficient to cause formation of the lactone. The other possibilities include cyclization during supercritical fluid extraction of the SOA from the filter samples, elution through the column of the gas chromatograph, and cyclization in the mass spectrometer. Because the gas chromatograph retention times of the sample lactones and the authentic standards were close, indicating a match, it is likely that the cyclization occurred either in the particle phase, during sample extraction, or elution through the GC column. Standards of γ-hydroxycarboxylic acids are generally not available and the step at which cyclization occurs cannot yet be determined and is a subject for future investigation.

Cyclization in the particle-phase, the oxidation processes resulting in dihydro-5-propyl-2(3H)-furanone and dihydro-5-pentyl-2(3H)-furanone and their corresponding γ-hydroxycarboxylic acid precursors, is proposed in Figure 4.10. The γ-hydroxycarboxylic acid can be derived from OH attack on the alkene. Following the initial hydroxyl radical attack on the alkene, oxygen rapidly adds to the alkyl radical resulting in an alkylperoxy radical. Nitric oxide is converted to nitrogen dioxide and the alkylperoxy radical to an alkoxy radical. A 1,5-hydrogen shift creates a new dihydroxyalkyl radical which subsequently reacts with oxygen and with nitric oxide to a dihydroxyalkoxy radical. Another 1,5-hydrogen shift creates a trihydroxyalkyl radical which rapidly adds oxygen to yield a trihydroxyalkylperoxy radical. This radical then reacts with nitric oxide to become a trihydroxyalkoxy radical. The alkoxy radical rearranges and loses CH_2OH to yield the γ-hydroxycarboxylic acid. The recent work of Kwok *et al.* (1996ab) of potentially identifying β-hydroxycarbonyls from the isomerization of β-hydroxyalkoxy radicals is consistent with these mechanisms. Figures 4.11 and 4.12 outline a possible course by which dihydro-5-ethyl-2(3H)-furanone and dihydro-5-methyl-2(3H)-furanone are formed from 1-octene. The corresponding analogs for 1-decene were not definitively identified.

Figures 4.11 and 4.12 are similar to Figure 4.10 with respect to the sequence of a 1,5-hydrogen shift and oxygen addition.

As suggested earlier, the role of higher alkenes in the atmosphere is important, not only with respect to ozone formation but also secondary organic aerosol formation. Comprehensive studies of the composition of urban organic aerosol at a molecular level have been conducted (Mazurek *et al.*, 1989; Rogge *et al.*, 1993). Over 80 organics from various classes (*i.e.*, *n*-alkanes, *n*-alkanoic acids) were quantified. Octanoic acid, nonanoic acid, decanoic acid, and nonanal were identified. In addition to primary sources, the photooxidation and subsequent gas-to-particle conversion of the reaction products of 1-octene, 1-nonene, and 1-decene could contribute to these ambient levels.

Conclusions

The composition of secondary organic aerosol from the NO_X-air photooxidation of 1-octene and 1-decene has been investigated. The dominant species in 1-octene aerosol were heptanal, heptanoic acid, and dihydro-5-propyl-2(3H)-furanone. The corresponding species in 1-decene aerosol were nonanal, nonanoic acid, and dihydro-5-pentyl-2(3H)-furanone. Gas-phase mechanisms of the reactions of 1-octene/1-decene with ozone, nitrate radicals, and hydroxyl radicals have been proposed leading to these products. The mechanisms were outlined generally, and R can be extended (*i.e.*, R=H to C_nH_{2n+1}) to include higher 1-alkenes. The reactions leading to the dominant species in the 1-octene/1-decene aerosol are summarized in Figure 4.13.

Appendix: Extraction of Secondary Organic Aerosol Components Using Supercritical CO_2

In this study, secondary organic aerosol (SOA) was collected on quartz fiber filters for subsequent molecular composition analysis via gas chromatography and mass spectrometry. It was determined that liquid solvent extraction may not be the optimal method to recover SOA species. Because traditional solvent techniques often necessitate concentration of solvent volumes from several hundred milliliters (ml) to volumes of tens of microliters (μl) via evaporation of the solvent, significant loss of SOA could result.

In recent years, supercritical fluid extraction (SFE), usually with CO_2 and a co-solvent, has received increased attention as a replacement for conventional liquid solvent extractions (Camel *et al.*, 1993; Hawthorne *et al.*, 1993; Janda *et al.*, 1993). Comparison between Soxhlet extraction, thermal desorption, other solvent methods, and SFE, have demonstrated SFE to be a viable alternative (Camel *et al.*, 1993; Hansen *et al.*, 1995; Furton and Rein, 1992). A further advantage of SFE is its ease to couple directly to various analytical instruments including gas chromatography, liquid chromatography, and supercritical fluid chromatography (Janda *et al.*, 1993; Hansen *et al.*, 1995).

Development of a method to extract secondary organic aerosol from quartz fiber filters utilizing supercritical fluid extraction is described here. The supercritical fluid extractor manufactured by the Suprex Corporation was employed in this study. The Suprex instrument can operate in an off-line mode, in which it collects the sample into a vial containing a small aliquot of solvent, or it can operate in an on-line mode in which it passes the sample directly to an analytical instrument. A comparison of the off-line and on-line sample collection methods was performed, as well as an optimization of key operating parameters, as suggested in the literature (Furton and Rein, 1992; Knipe *et al.*, 1992; Levy *et al.*, 1992; Foley and Crow, 1992): temperature of the supercritical CO_2, pressure, choice of co-solvent (or modifier) to use with the supercritical CO_2, quantity of modifier,

and extraction duration. Filters were impregnated with a standard solution of typical gas-phase photooxidation products, and then were used in the extractions for the off-line and on-line comparisons. Although it has been reported that recoveries from impregnated filters or other impregnated sample media are not adequate indicators of extraction efficiencies from actual environmental samples (Hawthorne *et al.*, 1993), the comparison of recoveries did provide information on the effectiveness of the technique. Conditions with the best overall extraction efficiencies were found to be achieved using the supercritical fluid extractor in the on-line mode, coupled directly to the GC with the CO_2 at 150 °C, 420 atm, with 2% modifier of 10% acetic acid in methanol.

Experimental

Chemicals and Instrumentation. All organics used in the standards and extraction testing procedures were obtained from Fluka Chemical Corp. (Ronkonkoma, NY), Aldrich Chemical Co. (St. Louis, MO), EM Science (Gibbstown, NJ), and Fisher Scientific (Fair Lawn, NJ), and were used as received. Supercritical Fluid Extraction/Chromatography (SFE/SFC) grade CO_2 was purchased from Air Products and Chemicals Inc. (Long Beach, CA). Quartz fiber filters from the Pallflex Products Corp. (Putnam, CT) were used.

The Suprex Corporation (Pittsburgh, PA) supercritical fluid extractor consists of three parts: the PrepMaster, AccuTrap, and a modifier pump (Levy, 1991; Ashraf-Khorassani *et al.*, 1992). The PrepMaster houses the oven in which the extraction cell is placed, and also the two pumps for the CO_2. The oven is rated to 150 °C and the pumps are capable of pressurizing the extraction cell to 500 atm. A variety of extraction cell volumes are available, from 0.5 ml to 50 ml. The 3 ml cell was used in this study. The modifier pump works in conjunction with the PrepMaster by supplying a prescribed amount of solvent to the extraction cell in order to modify the effective polarity of the supercritical CO_2. The

PrepMaster can be operated in a static or dynamic mode. In the static mode, the sample is pressurized with CO_2 and held at a constant temperature and pressure for a given amount of time. In the dynamic mode, CO_2 continually flows through the extraction cell for given amount of time at a particular temperature and pressure. The CO_2 and analytes can then be collected on-line or off-line. In the on-line mode, the CO_2 with the analytes can pass through a heated, stainless steel line directly to the injection port of the GC. The GC cryogenically collects and focuses the sample in the first meter of a capillary GC column maintained at -30 °C. The AccuTrap is used for off-line collection. The AccuTrap consists of a heated restrictor through which the CO_2 and analytes expand from extraction pressures to atmospheric pressure. After the restrictor, the CO_2 along with the analytes pass over a bed of glass beads. This bed can be maintained at temperatures from -40 to 60-°C. At the end of the extraction, the bed is washed with a prescribed quantity of a given solvent. The solvent and analytes are collected into a vial.

A Hewlett Packard (HP) 5890 Series II gas chromatograph equipped with electronic pressure control, and a 5989A mass spectrometer engine were used for detection and quantitation of recoveries for the SFE studies. Separation of standards was achieved using an HP-5MS 30m x 0.25 mm internal diameter capillary column with a phase thickness of 0.25 μm of 5% phenylmethylsiloxane. For the on-line studies, the temperature programming of the gas chromatograph consisted of maintaining an injection temperature of 210 °C, holding the oven at -30 °C during extraction, and then increasing to 250 °C. The GC/MS interface was maintained at 250 °C. The MS analyses were performed by electron impact ionization. The GC/MS was typically calibrated every two extractions. Quantitation with the mass spectrometer had probable errors ±27% of the value. For example, for an average recovery for a given set of extraction conditions of 85%, this value is more precisely represented as 0.85±0.21, and hence average extraction efficiencies over 80% were considered sufficient. It is important to note that, although a particular

temperature, pressure, and modifier were prescribed, small deviations (less than ±5%) from these set-points will still result in adequate recoveries of samples.

Procedure for Recovery Studies by SFE. The quartz fiber filters were impregnated with aliquots ranging from 5 to 50 µl of an organic standard. The standard solution contained an approximate concentration of 1 mg ml^{-1} each in methanol: butyl ester of nitric acid, heptanal, hexanoic acid, nonanal, 2-ethylhexyl nitrate, 2-nitro-*m*-xylene, benzoic acid, 5-nitro-*m*-xylene, undecanal, decanoic acid, pentanedioic acid, hexanedioic acid, dodecanoic acid, and tetradecanoic acid (Forstner, 1996). The filters were extracted immediately after spiking. Compound responses were compared to those from equivalent volume on-column injections of the standard. After each extraction, the SFE cell was cleaned by extracting the empty cell for 30 min at 120 °C and 450 atm. The cleanliness of the system was then verified before each sample extraction.

Results

Off-line studies. Prior to optimizing the operating parameters of the supercritical fluid extractor for maximal recovery, the method of sample collection was verified (Suprex Corporation, 1994). A comparison of the off-line (*i.e.,* AccuTrap) and on-line (*i.e.*, heated transfer line to gas chromatograph) sample collection methods was performed. The AccuTrap was first tested to determine its efficiency in collecting the species in the standard solution. The bed of glass beads in the AccuTrap was impregnated with 50 µl of the standard. Initially, the choice of collection solvent and desorption temperature were considered (Langenfeld *et al.*, 1992; Suprex Corporation, 1994). Other parameters include the volume of collection solvent, the rate at which the collection solvent passes over the trap, and the collection temperature during extraction. Since all compounds were considered as equally important, the optimal extraction conditions were considered to be those that result in the best possible overall extraction efficiency. Because recoveries of the

standard from the trap alone without extraction were poor, typically 30% or less, it was decided that no further studies utilizing off-line collection would be performed.

On-line studies. The following parameters were optimized to obtain the best recoveries: temperature, pressure, choice of modifier, flow rate of modifier to the extraction cell, and extraction duration (Camel *et al.*, 1993; Furton and Rein, 1992; Knipe *et al.*, 1992; Levy *et al.*, 1992; Suprex Corporation, 1994). Once the ranges of temperature and pressure were identified, a simplex approach was used to fine tune the temperature and pressure (Foley and Crow, 1992).

The effect of extraction duration on recoveries was initially compared. It was found that varying the times the instrument was held in its static mode had no effect on the recoveries. The duration of the dynamic extraction, however, was found to have significant effect on the extraction efficiencies. For each extraction, two quartz fiber filters impregnated with 50 µl of standard were extracted at 140 °C, 400 atm., with a modifier of 10% acetic acid in methanol added to the cell at 2% the flow rate of the CO_2. Reasonable extraction efficiencies were obtained with a 30 min dynamic extraction.

Recoveries from three extractions with different pressures were compared. For each pressure, 50 µl of the standard was extracted from a quartz fiber filter at 80 °C with a 10% acetic acid in methanol modifier being added to the extraction cell at 10% of the CO_2 flow rate. The best recoveries were achieved at the higher pressure of 400 atm. A series of extractions with varying temperatures were also performed to determine an optimal temperature. Again, 50 µl of standard was extracted at 400 atm with 10% acetic acid in methanol modifier added to the cell at a rate of 10% of the CO_2 flow rate. Better recoveries were achieved at higher temperatures. Based on the comparison of collection solvents in the off-line studies, the effectiveness of methanol, ethanol, isopropanol, ethyl acetate, and 10% acetic acid by volume in methanol, as modifiers, was studied. The modifier for further extractions was chosen to be the solution of 10% acetic acid by volume in methanol

in order to adequately recover organic acids from quartz fiber filters. Once the basic conditions of the system were determined, a simplex approach was used to narrow the temperature and pressure ranges for optimal extraction efficiencies. Quartz fibers filters were impregnated with very small aliquots of 5 μl of the standard. The optimal conditions were chosen to be 420 atm, 150 °C, with 2% modifier of 10% acetic acid by volume in methanol. The extraction had a static mode of 10 min and then 30 min dynamic mode. Table 4.5 lists the fractional recoveries for each compound in the standard, extracted at these optimal conditions.

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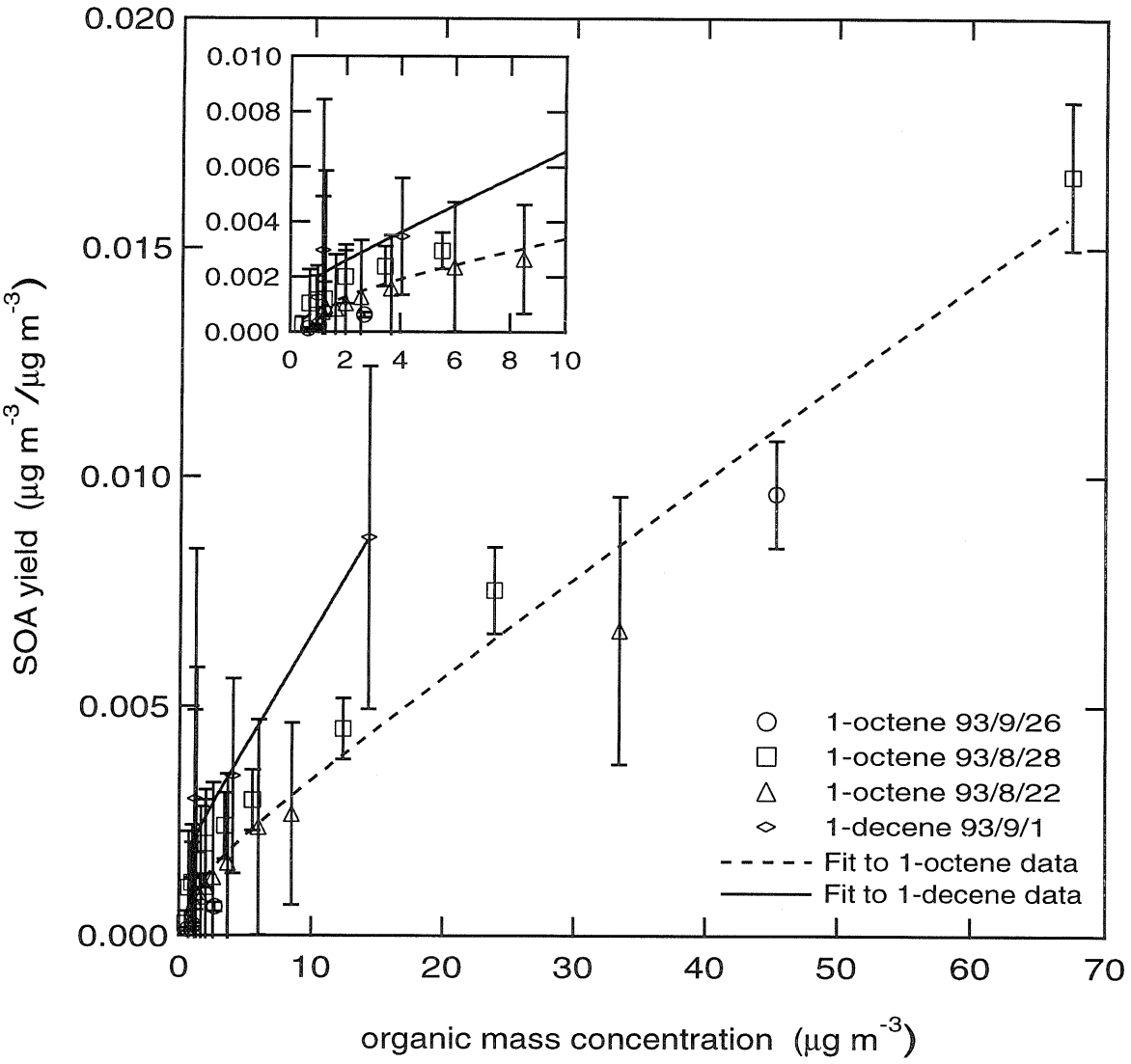

Figure 4.1 Time dependent SOA yields of individual 1-octene and 1-decene experiments as a function of organic mass concentration ($M_O(t)$). The production of secondary organic aerosol is controlled by an equilibrium partitioning of semi-volatile compounds between the gas-phase and organic matter phase, described by equation (1). A two-product model of equation (1) was fitted to the experimental data. Dates of experiments indicated (see Table 4.1).

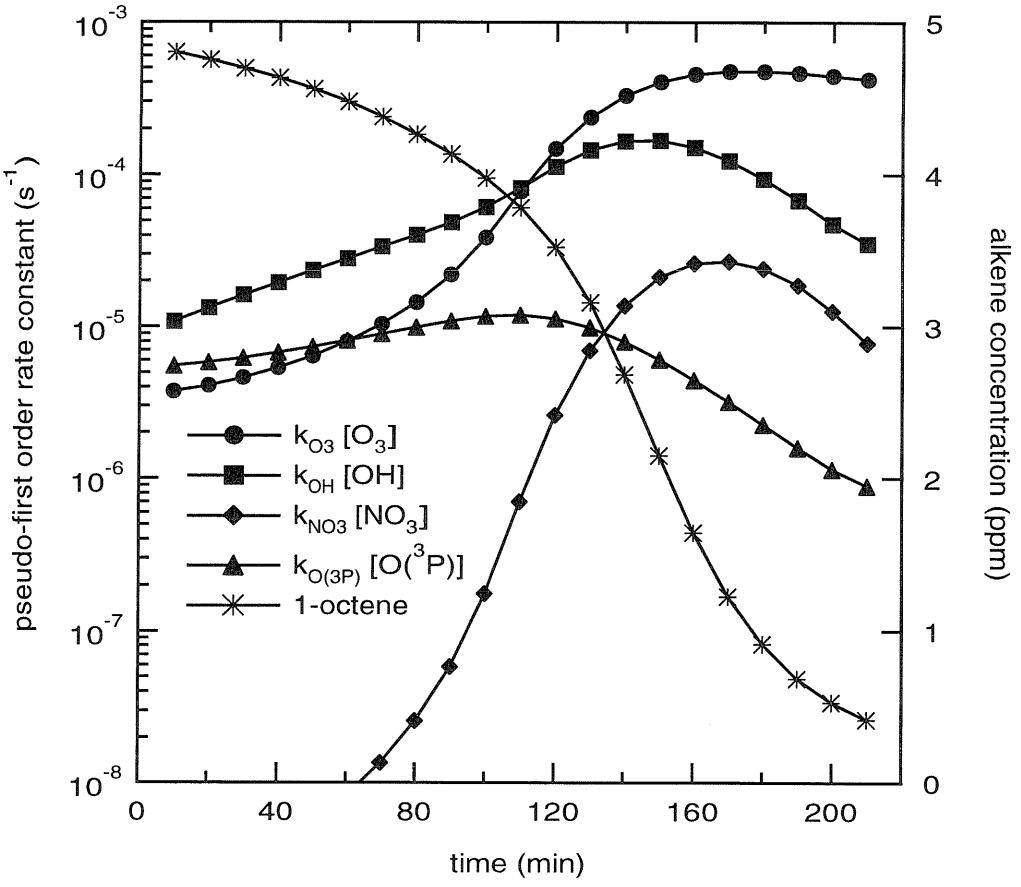

Figure 4.2. Comparison of pseudo-first order rate constants for OH, NO_3, O_3 and $O(^3P)$ for 22 August 1-octene experiment.

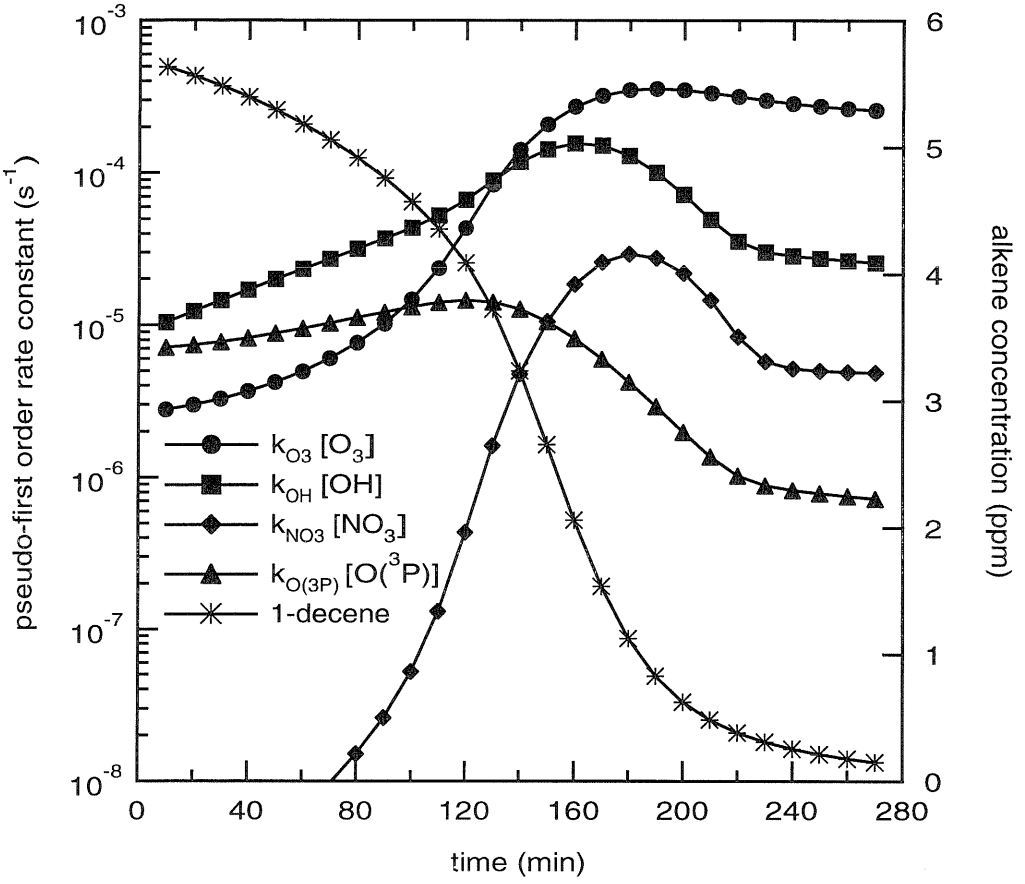

Figure 4.3. Comparison of pseudo-first order rate constants for OH, NO_3, O_3 and $O(^3P)$ for 30 August 1-decene experiment.

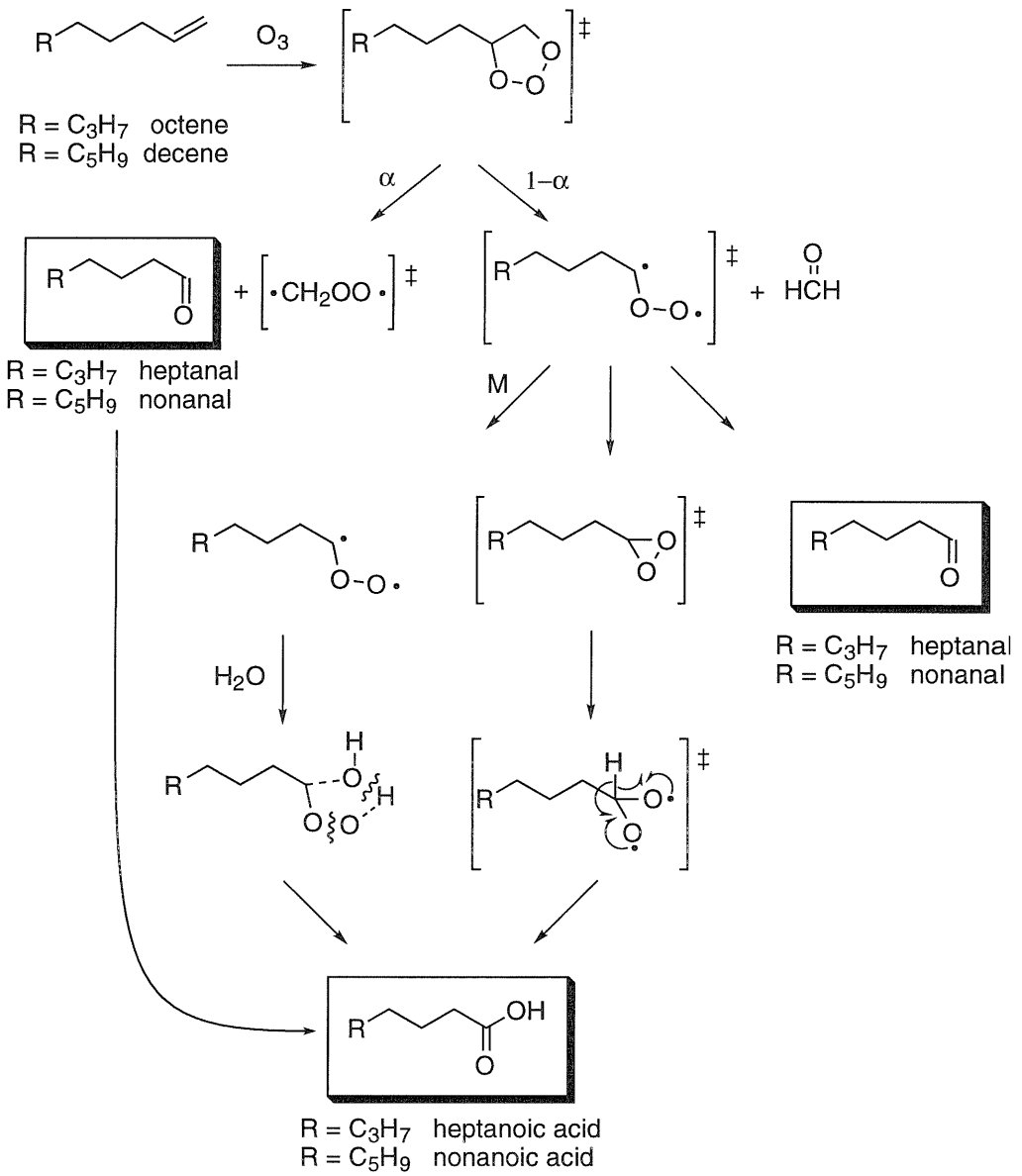

Figure 4.4. Mechanism of O3 addition to 1-octene/1-decene leading to heptanal/nonanal.

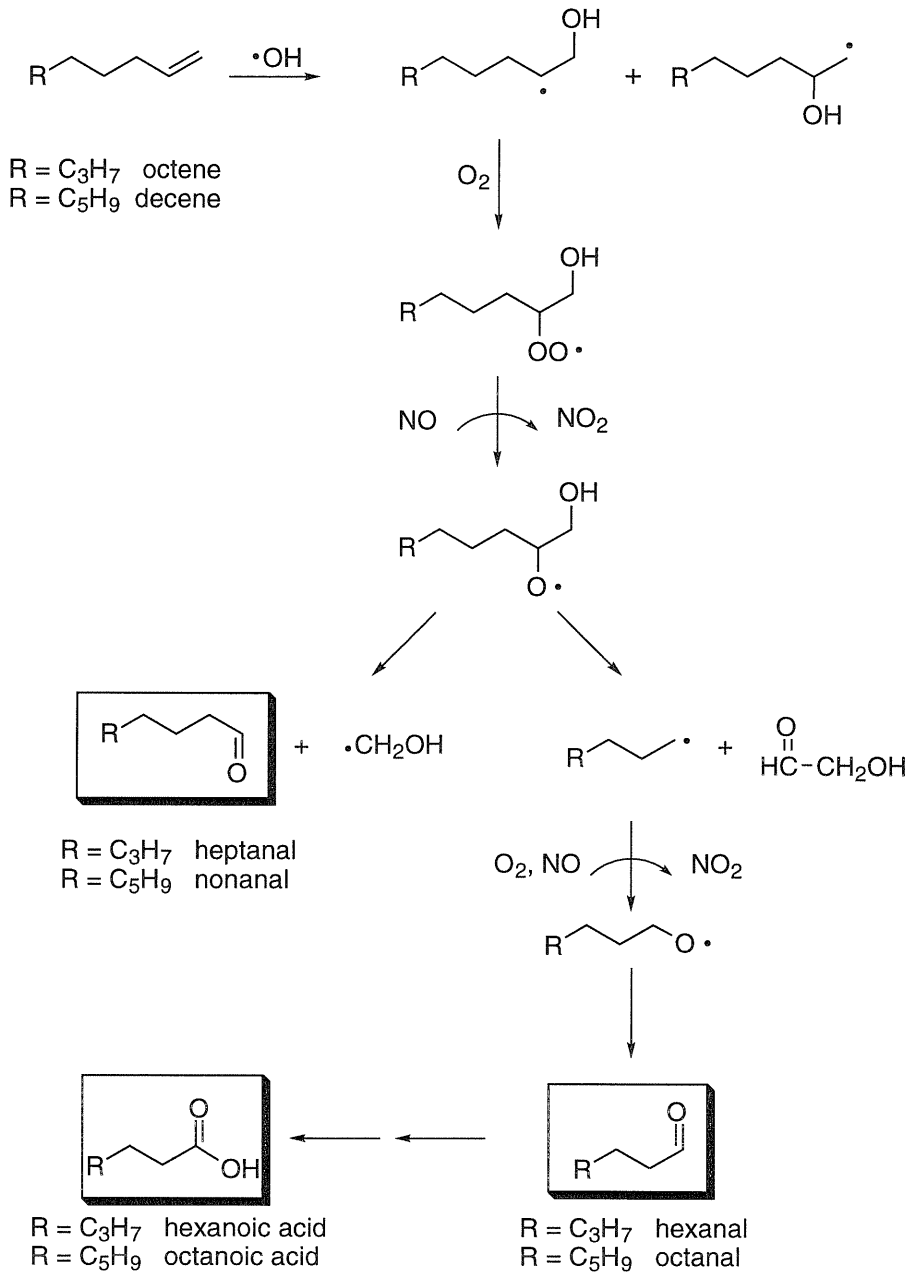

Figure 4.5. 1-Octene-/1-Decene-OH pathway leading to heptanal/nonanal and hexanal/octanal.

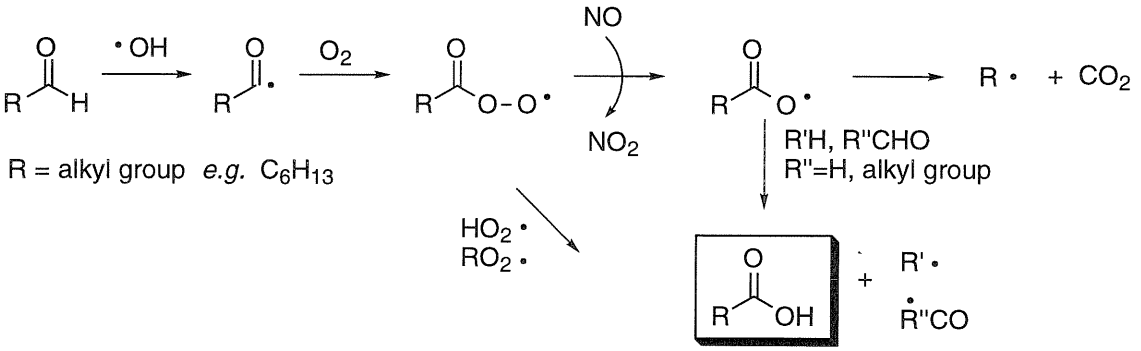

Figure 4.6. Mechanism of aldehyde oxidation to its carboxylic acid.

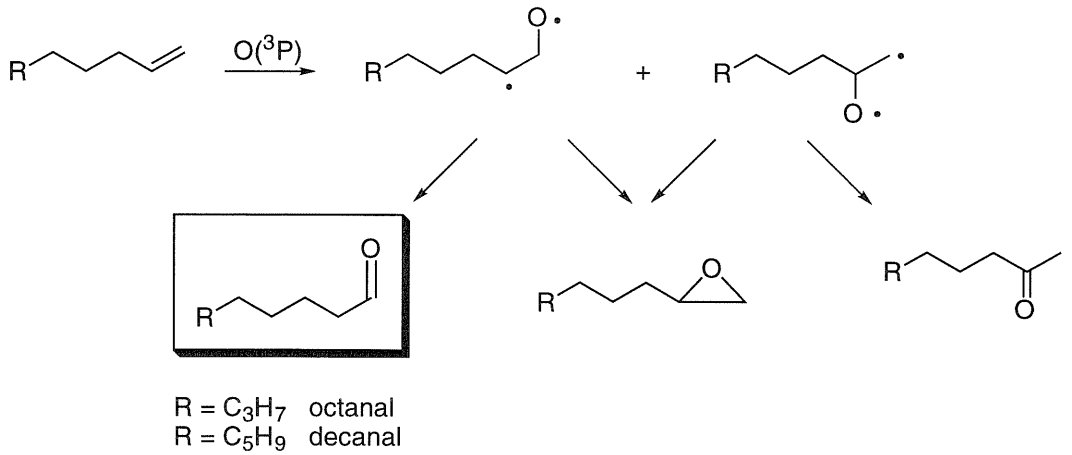

Figure 4.7. 1-Octene/1-Decene-O(^{3}P) pathway leading to octanal/decanal.

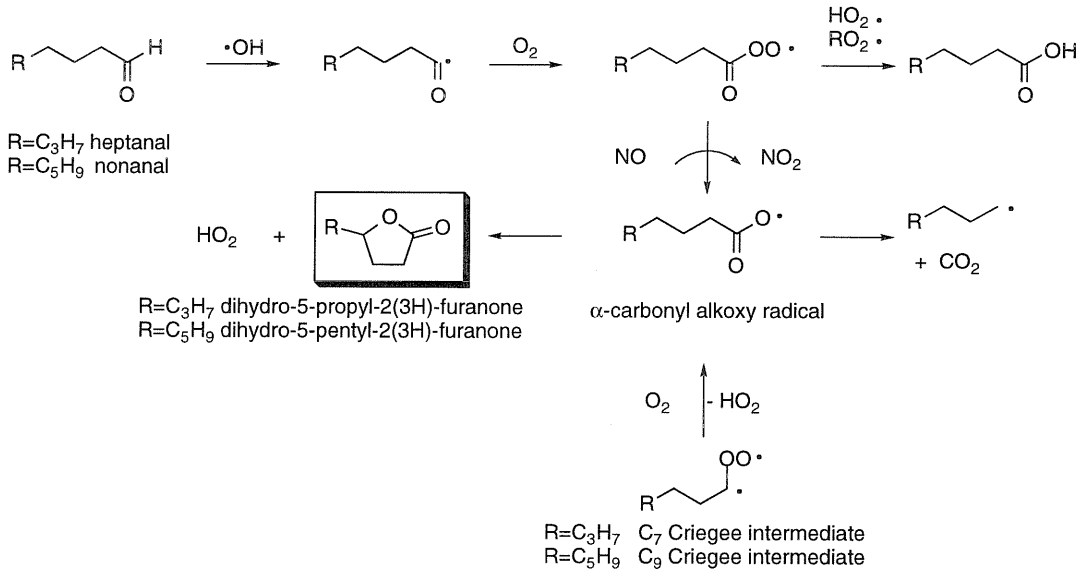

Figure 4.8. Possible mechanism leading to dihydro-5-propyl-2(3H)-furanone and dihydro-5-pentyl-2(3H)-furanone from heptanal and nonanal (Wang *et al.*, 1992).

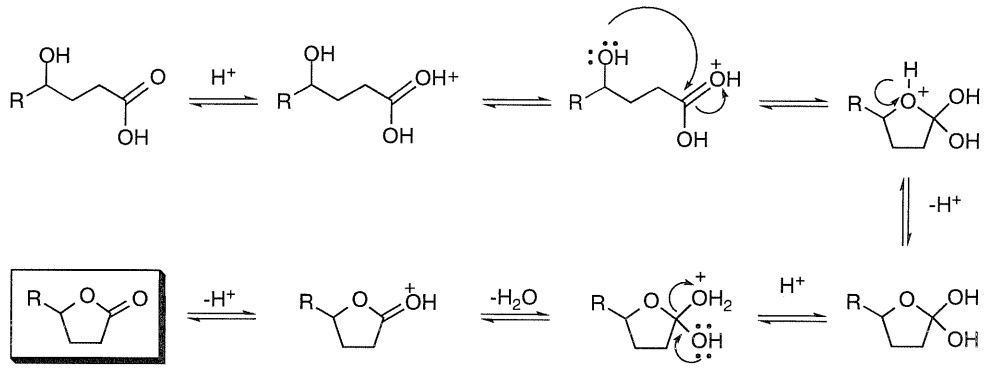

Figure 4.9. Cyclization of γ-hydroxycarboxylic acid to its lactone (Streitwieser and Heathcock, 1976).

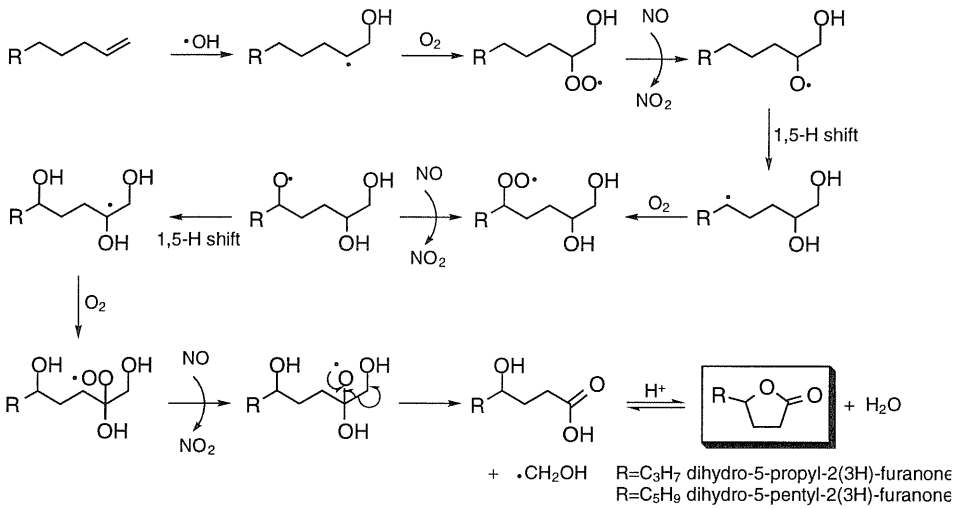

Figure 4.10. 1-Alkene-OH pathway leading to γ-hydroxycarboxylic acid and its lactone.

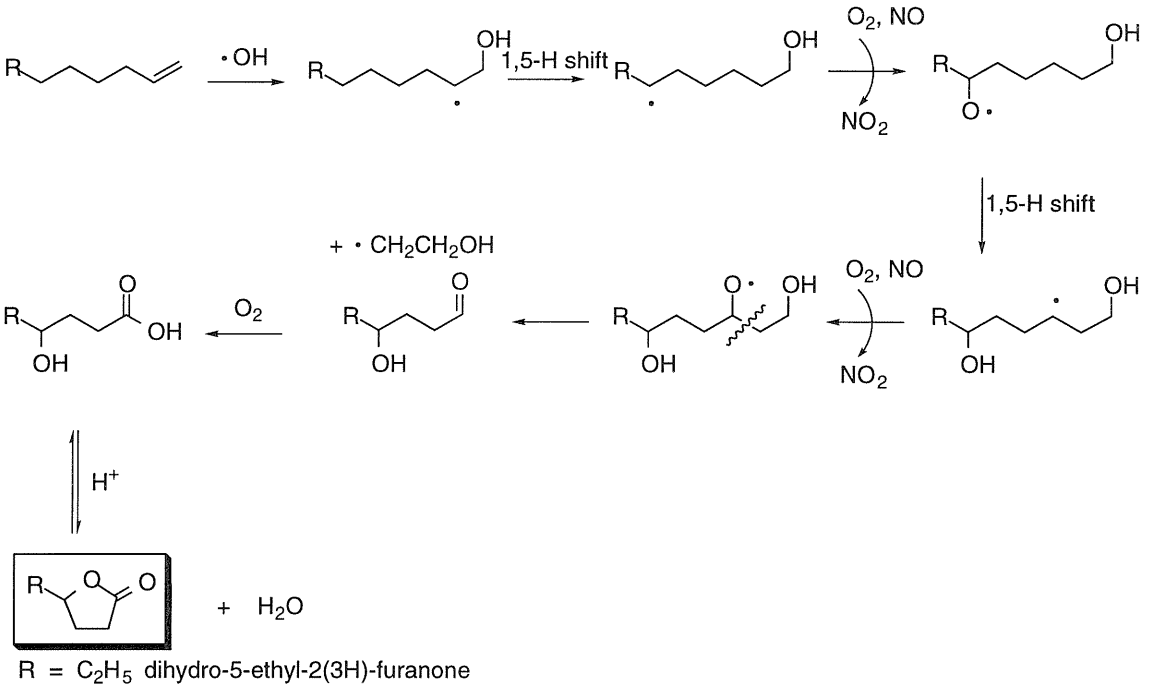

Figure 4.11. 1-Octene-OH pathway leading to dihydro-2-ethyl-2(3H)-furanone.

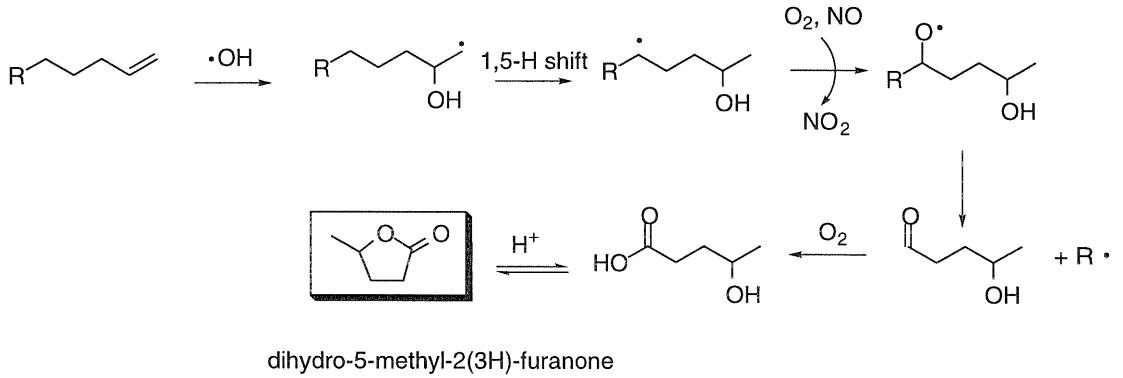

Figure 4.12. 1-Octene-OH pathway leading to dihydro-5-methyl-2(3H)-furanone (R=C3H7).

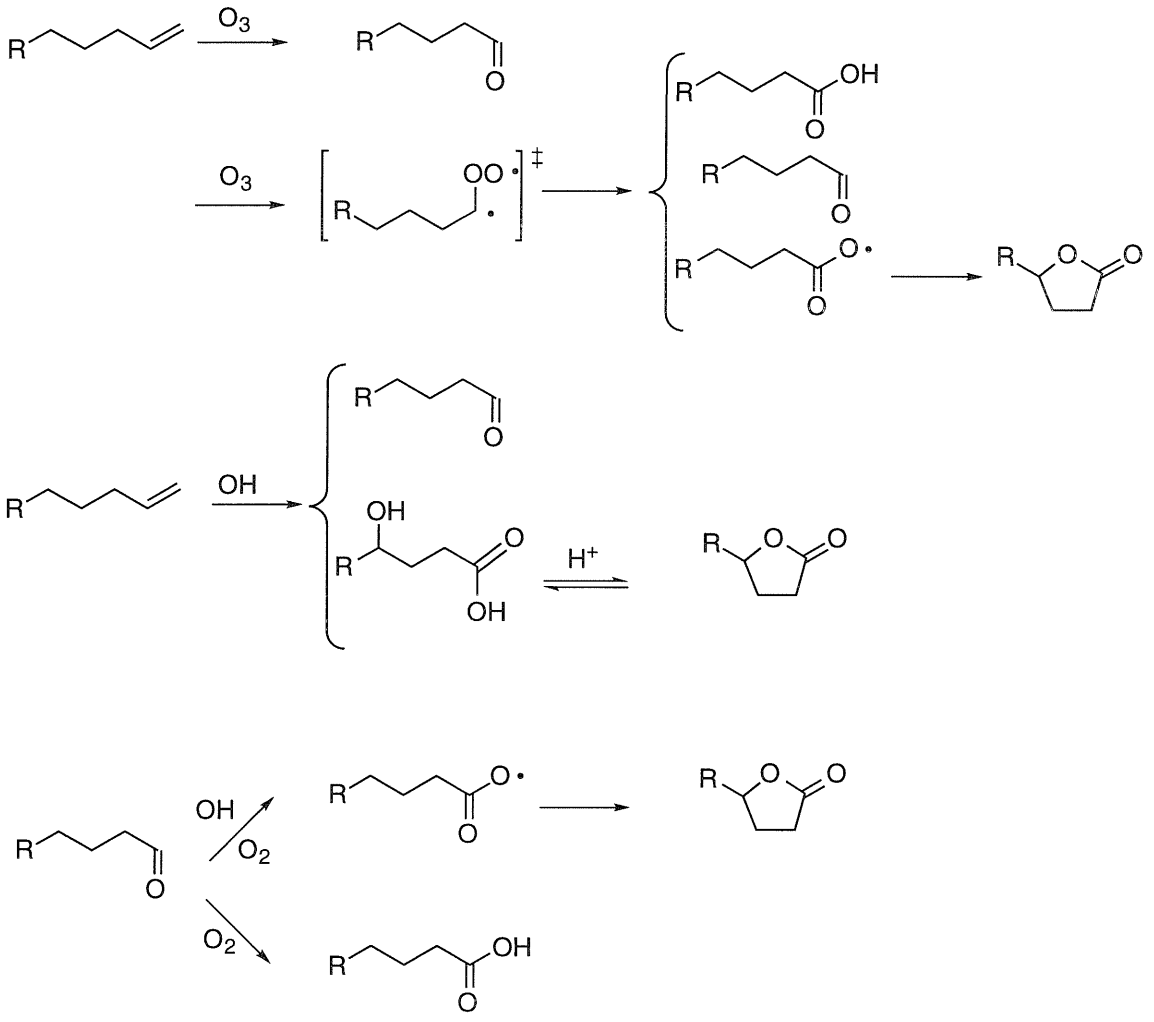

Figure 4.13. Summary of gas-phase 1-alkene-OH and 1-alkene-O3 reactions leading to predominant products in aerosol.

Table 4.1. Initial conditions of outdoor smog chamber experiments.

	date	HC ppm	NO ppb	NO_2 ppb	NO_X ppb	HC/NO_X ratio ppbC/ppb	particles N_o # cm^{-3}
1-octene	8/22/93	4.8	987	452	1439	27	840
	8/28/93	5.6	852	446	1298	34	510
	9/26/93	2.6	687	314	1001	21	460
1-decene	8/30/93	5.7	1202	603	1805	32	1100
	9/01/93	5.7	1171	649	1820	31	450
	9/03/93	6.0	1298	643	1941	31	260
	10/25/93	2.7	773	368	1141	23	690

Table 4.2. Fraction of total identifiable organic mass in 1-octene SOA.

organics	93-8-22	93-8-28	93-9-26	density g cm^{-3}
heptanal	0.375	0.227	0.325	0.818
heptanoic acid	0.266	0.321	0.222	0.918
dihydro-5-propyl-2(3H)-furanone	0.250	0.293	0.346	~1
hexanal	0.036	†	0.033	0.834
dihydro-5-ethyl-2(3H)-furanone	0.031	0.028	0.030	1.027
dihydro-5-methyl-2(3H)-furanone	0.017	0.088	0.024	1.057
1-nitrohexane	0.006	†	0.005	0.940
dihydro-2(3H)-furanone	0.006	0.005	0.009	1.120
1-hexanol	0.005	†	0.003	0.814
octanoic acid	0.003	0.031	not detected	0.910
octanal	0.002	†	not detected	0.821
hexanoic acid	0.002	0.007	0.004	0.927

†Detected and verified, but at levels too low to accurately quantify.

Table 4.3. Fraction of total identifiable organic mass in 1-decene SOA.

organics	**93-8-30**	**93-9-1**	**93-9-3**	**93-10-25**	**density** g cm^{-3}
nonanal	0.431	0.406	0.442	0.413	0.827
nonanoic acid	0.252	0.253	0.283	0.073	0.916
dihydro-5-pentyl-2(3H)-furanone	0.134	0.187	0.105	0.443	0.976
octanal	0.053	0.052	0.053	not detected	0.821
decanal	0.035	0.019	0.017	0.002	0.830
decanoic acid	0.032	0.025	0.025	0.036	0.893
dihydro-5-propyl-2(3H)-furanone	0.015	0.014	0.011	0.008	~1
heptanoic acid	0.011	0.007	0.006	not detected	0.918
heptanal	0.008	†	†	†	0.818
2-heptanone	0.007	0.004	0.002	not detected	0.820
hexanal	0.006	†	0.020	†	0.834
dihydro-5-ethyl-2(3H)-furanone	0.005	0.007	0.006	0.005	1.027
octanoic acid	0.005	0.009	0.011	0.021	0.910
1,2-epoxyoctane	0.004	0.013	0.017	not detected	0.839
1-octanol	0.002	0.003	0.004	0.001	0.827

†Detected and verified, but at levels too low to accurately quantify.

Table 4.4. Rate constants at 298K (cm^3 $molecule^{-1}$ s^{-1}).

	1-octene	1-decene
k_{OH}	4.0×10^{-11} †	3.7×10^{-11} ‡
k_{O3}	1.7×10^{-17} †	1.2×10^{-17} ‡
k_{NO3}	1.2×10^{-14} ‡	1.2×10^{-14} ‡
$k_{O(3P)}$	4.2×10^{-12} †	4.2×10^{-12} ‡

† (Paulson and Seinfeld, 1992)

‡ (Carter, 1990)

Table 4.5. Fractional recoveries of standards using supercritical fluid extraction.

standard	recovery
butyl ester of nitric acid	0.33
heptanal	0.96
hexanoic acid	0.95
nonanal	0.92
2-ethylhexyl nitrate	0.86
2-nitro-m-xylene	0.91
benzoic acid	0.85
5-nitro-m-xylene	0.84
undecanal	0.91
decanoic acid	0.91
pentanedioic acid	0.70
hexanedioic acid	0.73
dodecanoic acid	0.90
tetradecanoic acid	0.88

CHAPTER 5

CONCLUSIONS

The first part of this work involves investigation of the physical aspect of secondary organic aerosol (SOA) formation. Outdoor smog chamber experiments were performed to compare aerosol yields from the photooxidation of toluene, *m*-xylene, *p*-xylene, ethylbenzene, *m*-ethyltoluene, *p*-ethyltoluene, and 1,2,4-trimethylbenzene in the presence of NO_X. For all the aromatics, the aerosol yield was found to correlate with organic mass concentration according to semi-volatile gas/particle partitioning theory. Organic aerosol mass serves as the particulate-phase medium into which gas-phase species absorb. Therefore, the total amount of organic aerosol mass directly affects gas/particle partitioning. The greatest aerosol yields were attained from the C9 aromatics, and the smallest yields from toluene and ethylbenzene. These results provide a source of aerosol yield data that can be used by models predicting SOA formation.

The largest contribution of this research to understanding atmospheric aerosol formation is the molecular characterization of secondary organic aerosol from aromatic photooxidation. As noted in the Introduction, numerous studies have demonstrated the aerosol formation potential of the above aromatic compounds, but few studies have addressed the composition. The present study represents a comprehensive effort to determine the composition of aerosol from aromatic photooxidation. This aerosol is predominantly unsaturated anhydrides, such as 2,5-furandione, and 3-methyl-2,5-furandione. The presence of these compounds is consistent with the current understanding of the gas-phase mechanisms of aromatic-OH photooxidation leading to ring-fragmentation products. The most important contribution is the identification of saturated furandiones and alkyl diketones. Not only are these compounds not predicted

from current mechanisms, they have not been previously reported in gas-phase studies, suggesting the possibility of particle-phase, photo-hydrogenation of the corresponding unsaturated species. The knowledge of aerosol composition has provided insight into elucidating gas-phase mechanisms of aromatic photooxidation. It has also provided further support for the gas/particle partitioning theory as compounds not expected to condense based on their relatively high vapor pressures are detected in comparable, if not greater, quantities in the aerosol than species predicted to exist in the particle phase.

Additional outdoor smog chamber studies of octene and decene were performed to identify aerosol constitutents. The organics identified were consistent with the current understanding of alkene photooxidation. Finally, a novel sample preparation technique was developed to extract aerosol from filter samples using supercritical fluid CO_2. A series of tests using a standard known solution of organics was performed to optimize the extraction protocol.

This work demonstrates potential new areas of research in atmospheric aerosol formation. In gas/particle partitioning, the anomalies in the *m*-xylene curves of aerosol yield against organic mass need to be further investigated (Chapter 2). Since temperature was not a factor in the *m*-xylene experiments, it needs to be determined whether the discrepancies are due to: nucleation processes and hence a surface area effect; the assumptions of the model not holding in this particular case; or some other phenomena. It would be useful to complete the data set for all seven aromatics, by extending the range of organic mass concentrations for the aerosol yield correlations, and by determining partitioning coefficients.

The potential areas of research in SOA composition are great. The unidentified portion (~70-85%) of SOA for each aromatic needs to be identified. Along with SOA characterization, current understanding of gas-phase aromatic oxidation mechanisms is largely incomplete. Studies to further knowledge of ring-fragmentation pathways and the

corresponding products are necessary. As well, determination of gas-phase product yields of these ring-fragmentation reactions would be useful for atmospheric models which incorporate these yields and gas/particle partitioning coefficients to quantitatively predict SOA formation. Finally, the possible formation of unsaturated furanones and furandiones (*e.g.,* 2,5-furandione) from hydrogenation in the particle phase in sunlight needs to be further studied in order to verify suggested mechanism, and to determine other kinetic parameters such rate constants and product yields.

APPENDIX A

Aerosol Measurement: Data Inversion from the Scanning Electrical Mobility Spectrometer

The measurement of particle size distributions with particles less than 0.1 μm in diameter has been accomplished with electrical mobility methods. The first instruments, such as the electrical aerosol analyzer (EAA) and the differential mobility analyzer (DMA), required significant measurement times, on the order of minutes, to acquire a size distribution. Since aerosol dynamics in smog chamber systems can vary rapidly, particularly when nucleation occurs, a technique developed by Wang and Flagan (1990) was used to measure the particle size distributions in the smog chamber experiments. Wang and Flagan's scanning electrical mobility spectrometer (SEMS) permits high resolution measurement of fine particle distributions on the order of seconds. SEMS monitors the transmission of particles through a time-varying electric field in a differential mobility analyzer (DMA). A condensation nuclei counter (CNC) was used to count the transmitted particles. The TSI Model 3071 DMA and TSI Model 3760 CNC were used. Custom software was used to collect the data. A complete description of the technique and the theory involved can be found in Wang and Flagan (1990).

The DMA was operated similarly for all experiments presented. The flow of air through the DMA, termed the sheath flow, was approximately 16 L min^{-1}. The aerosol sample flow rate was dictated by the condensation nuclei counters and was approximately 1.5 L min^{-1}. The DMA voltage was exponentially increased from 40 to 9500 V, thereby scanning the particle size distribution from 12 to 200 nm in diameter. The SEMS software inverted the raw data to yield time-resolved particle size distributions (Wang and Flagan, 1990). The data inversion was simplified by assuming perfect instrument response and that particles carry only one charge. The Fuchs model was employed to

estimate the bipolar charge distribution (Fuchs, 1963). An example of a particle size distribution is shown in Figure A.1.

To better represent the data provided by the original SEMS software, new software was developed to account for more complex particle phenomena. The data from the DMA and CNC include particles greater than 100 nm in diameter. Particles smaller than 100 nm are mostly singly-charged, but larger particles often have multiple charges. The bipolar diffusion charging probability of particles of various diameters having none, one, or two negative or positive charges is shown in Figure A.2. As the particle diameter increases, the probability of multiple charges increases. As the particle diameter approaches 200 nm, the probability of two negative charges is 15%, while the probability of a 200 nm particle having one charge is only 25%. Multiply-charged particles on the size distribution are not accounted for in the original SEMS software. An algorithm was written to correct the SEMS inverted data for multiple-charging effects, and to update the Fuchs charge distribution. The inverted data was additionally corrected for particle losses in the DMA and for the CNC counting efficiency (Wang *et al.*, 1992; Wang and Flagan, 1990). The Wiedensohler approximation of the Fuchs distribution was employed (Wiedensohler, 1988). The algorithm to account for multiply-charged particles involved subtracting from the smaller size bins those particles with larger diameters but multiple charges. The algorithm considered up to four charges per particle. The algorithm yields reasonable results if the distribution does not grow too far beyond the upper limit of the DMA, *i.e.,* 200 nm. It was assumed that if the particle size distribution ends at 200 nm, those particles are mostly 200 nm in diameter and singly-charged, *i.e.,* multiply-charged, larger particles are not present. The distribution at the smaller size bins can then be adjusted to account for the doubly-charged, triply-charged, and quadruply-charged 200 nm particles. This process continues and next considers a smaller particle that is, for example, 198 nm in diameter, and corrects the smaller size bins for multiply-charged 198

nm particles. The size distribution in Figure A.1 is corrected using the above code and is shown in Figure A.3, along with the original data inversion of Figure A.1. The inversion code is included after the figures.

References

Fuchs N. A. (1963) On the stationary charge distribution on aerosol particles in bipolar ionic atmosphere. *Geofis. Pura. Appl.* **56**, 185-193.

Wang S. C. and Flagan R. C. (1990) Scanning electrical mobility spectrometer. *Aerosol Sci. Technol.* **13**, 230-240.

Wang S.-C., Paulson S. E., Grosjean D., Flagan R. C. and Seinfeld J. H. (1992) Aerosol formation and growth in atmospheric organic/NO_x systems-I. outdoor smog chamber studies of C_7- and C_8-hydrocarbons. *Atmospheric Environment* **26A**(3), 403-420.

Wiedensohler A. (1988) An approximation of the bipolar charge distribution for particles in the submicron size range. *J. Aerosol Sci.* **19**(3), 387-389.

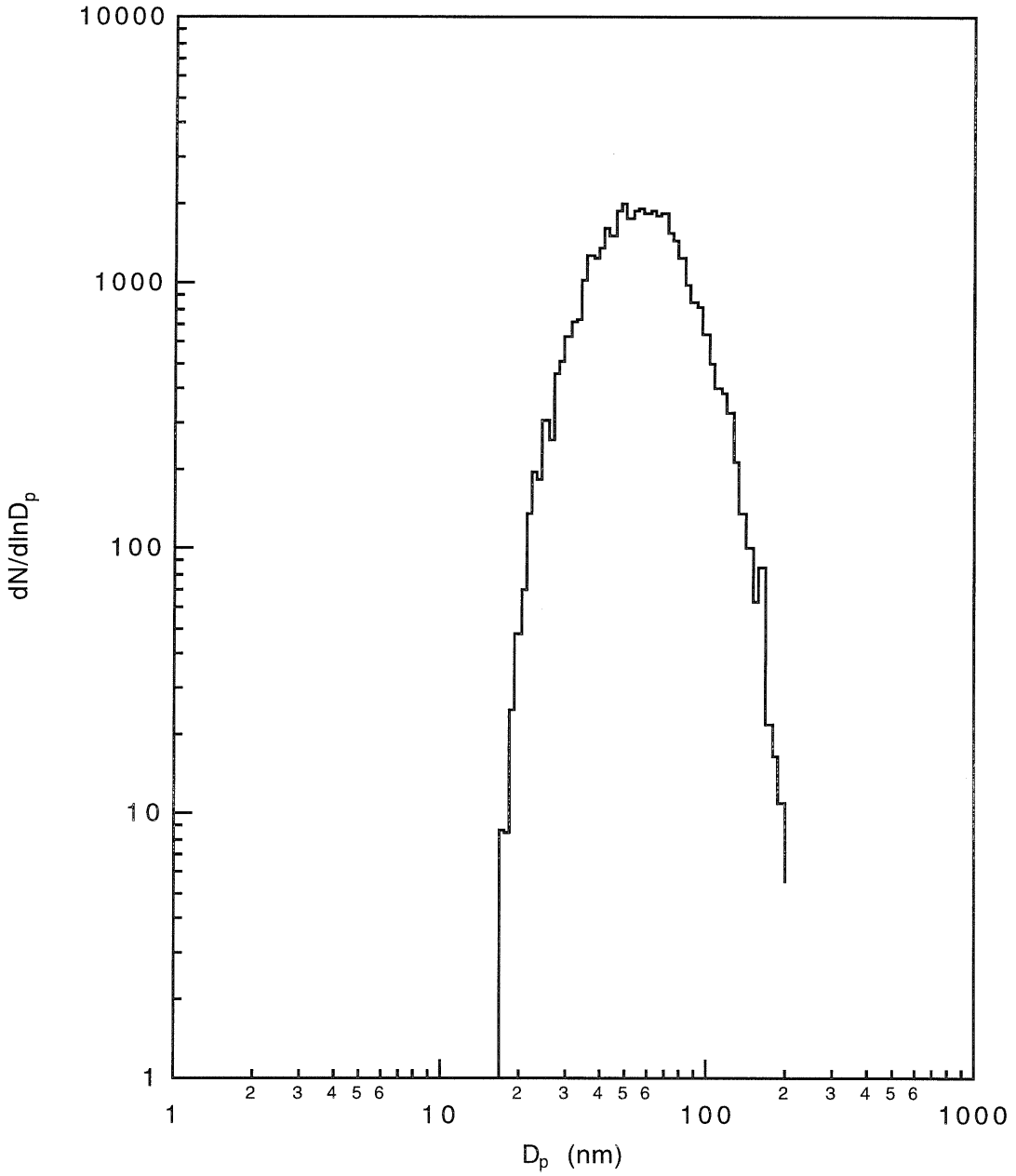

Figure A.1. Particle size distribution from SEMS.

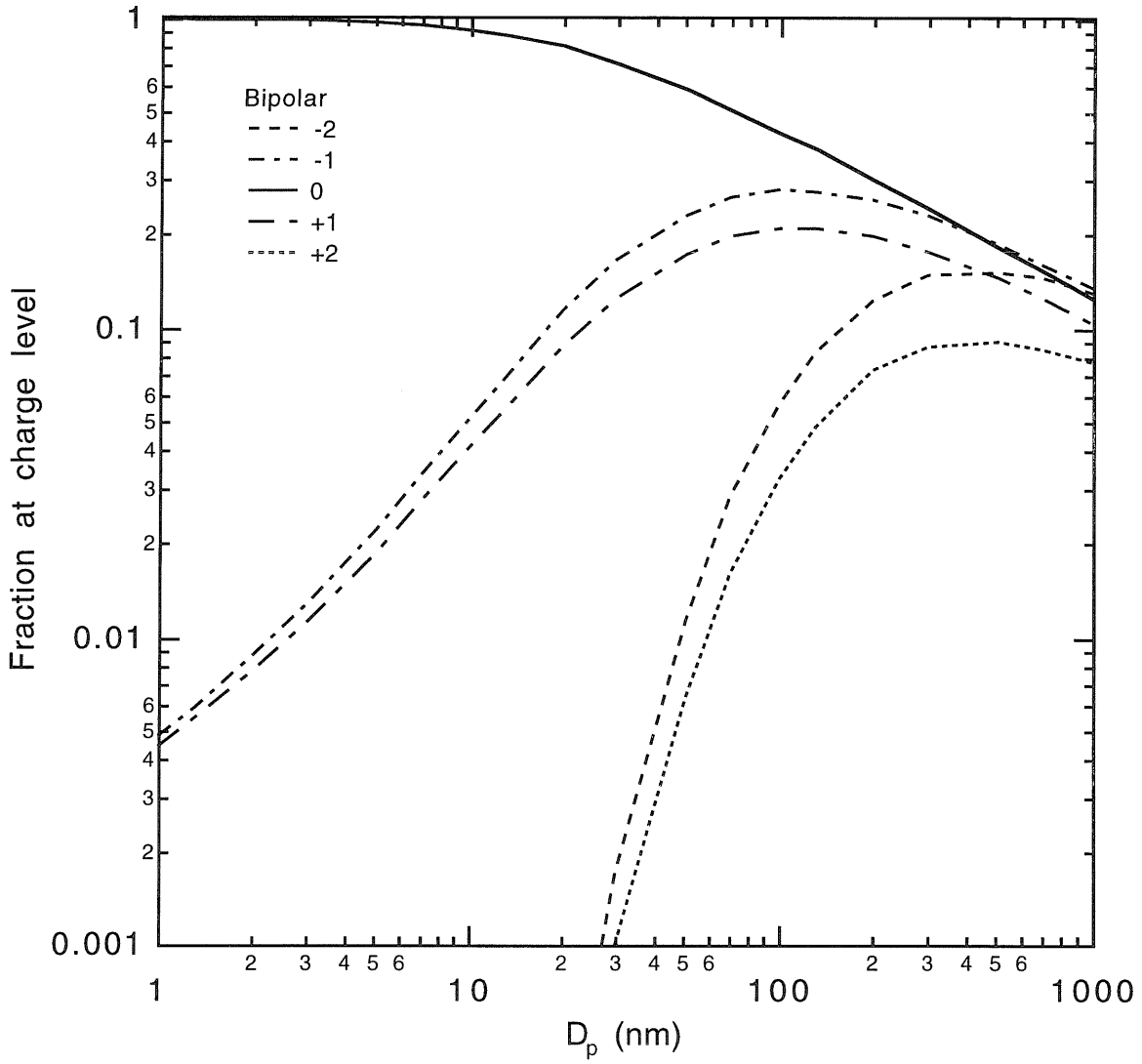

Figure A.2. Bipolar diffusion charging probability of particles.

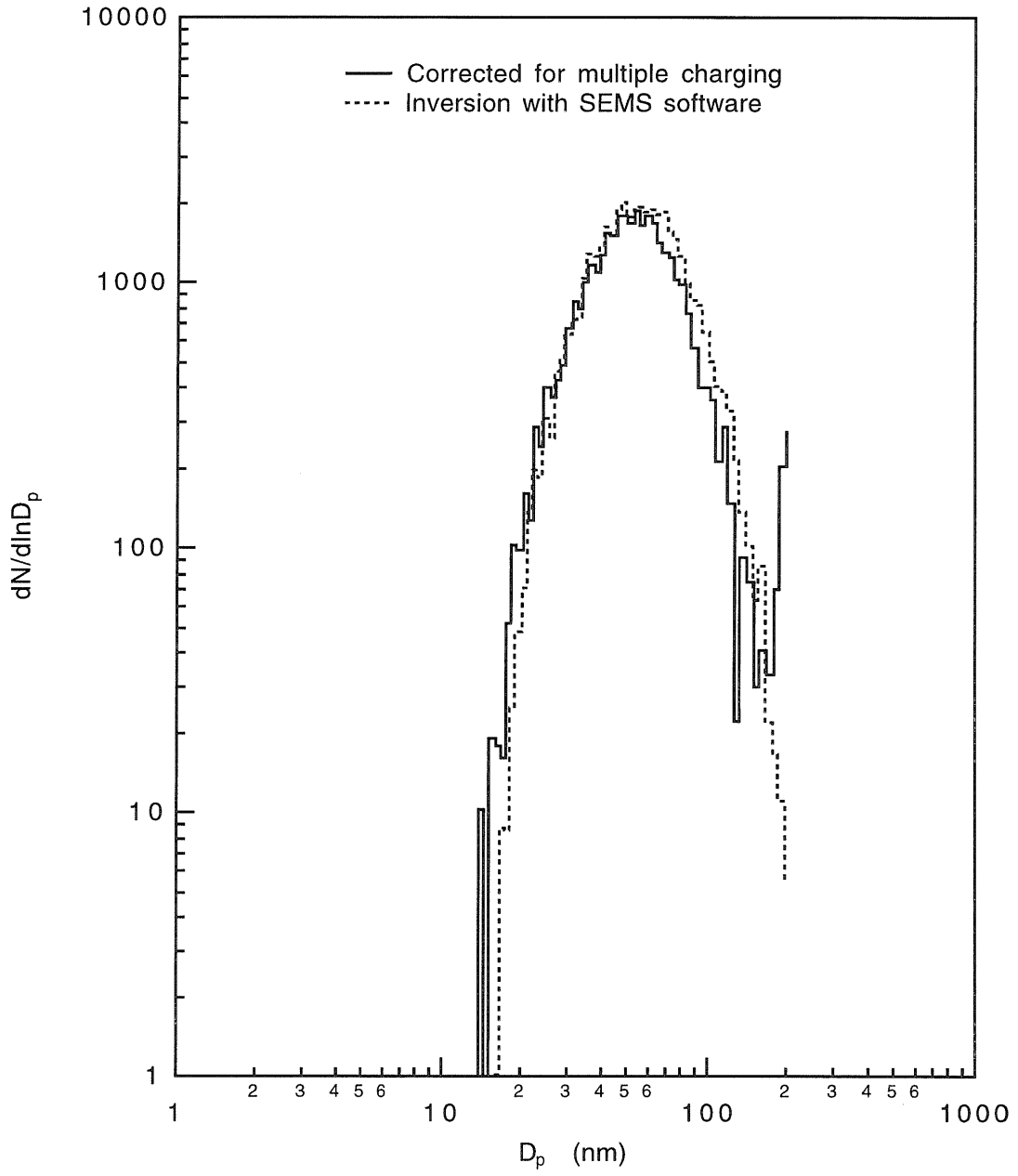

Figure A.3. Particle size distribution corrected for multiple charging compared with distribution from SEMS.

```
      Program SEMSINV2

c  ***********************************************************************
c  *****                                                     *****
c  *****   SEMSINV is a program to invert DMA data produced by the*****
c  *****   SEMS program.  Corrections are made for losses in the  *****
c  *****   DMAs and CNCs, and for multiple charging.  Originally  *****
c  *****   written by Frank Bowman 11/95, and modified by         *****
c  *****   Frank Bowman and HaliForstner, 4/96.                   *****
c  *****                                                     *****
c  *****   The command line is of the form:                  *****
c  *****                                                     *****
c  *****       SEMSINV dfile  atime                          *****
c  *****                                                     *****
c  *****   where dfile is the base name of the input data files,  *****
c  *****     dfile = series of raw data files                *****
c  *****                 (e.g. etbmet1a, etbmet1b,...)       *****
c  *****   and atime is the start time of the experiment         *****
c  *****     with the format HHMM, HH=hours, MM=minutes          *****
c  ***********************************************************************

      CHARACTER*8 DFILE,RUNFILE,ATIME
      CHARACTER*12 DIFILE,DRFILE,IFILE,RFILE,PFILE,XFILE
      CHARACTER*12 OAFILE,OBFILE,ONFILE
      CHARACTER*12 adum
      INTEGER DLEN,RLEN,TLEN,TH,TM,NM2,NM3,NM4,DEXT,EFLAG
      INTEGER HR,MIN,SEC,TIM(200),nm5,nm6
      REAL T0,PTNUM,TPC,TDC,CNCFCA,CNCFCB,TCOUNT,QMOC
      REAL T1,VTBL(100),D(120),IFACTORC(100),LOSS(120)
      REAL MCHRG(100,100),TSTART,SUMA(200),SUMB(200)
      REAL TEND,TAVE
      REAL DL,VA,VB
      REAL nlossa, nlossb, na, nb
           real ca(120),cb(120),sa,sb,dna(120),dnb(120)
      REAL DNTA(120,200),DNTB(120,200)
      REAL NTOTA(200),NTOTB(200),VTOTA(200),VTOTB(200)
           real SATOTA(200),SATOTB(200)
      REAL NTOTAc(200),NTOTBc(200),VTOTAc(200),VTOTBc(200)
           real SATOTAc(200),SATOTBc(200)


      REAL LD,RF,DEL

      REAL dum,dum1,dum2,dum3,timsec



c  ***** Read command line. Get base file names and start time *****


           write(*,*) 'Data file:'
           read(*,23) dfile
 23    format(a8)
           write(*,*) 'Start time:'
           read(*,23)          atime
c     dfile='etbmet1'
c     atime='0947'
```

```
          dlen=index(dfile, ' ')-1
          tlen=index(atime, ' ')-1
      write(*,*) dfile,atime,dlen,tlen

c          N=NARGS()
c     IF(N.NE.3)THEN
c       WRITE(*,*) ' ERROR: must specify datafile, runfile, time'
c       GOTO 999
c     ENDIF
c     CALL GETARG(1,DFILE,DLEN)
c     CALL GETARG(2,RUNFILE,RLEN)
c     CALL GETARG(2,ATIME,TLEN)
c     IF(DLEN.GT.6) DLEN=6
c     IF(RLEN.GT.7) DLEN=7
     IF(TLEN.NE.4)THEN
       WRITE(15,*) 'ERROR: time should be in HHMM form'
       GOTO 999
     ENDIF

c  ***** Assign input and output file names  *****

          difile=dfile
c     DIFILE=DFILE(1:DLEN)//'I'
c     DRFILE=DFILE(1:DLEN)//'R'
          ifile='loss.tbl'
c     IFILE='I'//RUNFILE(1:RLEN)
c     RFILE='R'//RUNFILE(1:RLEN)
c     PFILE='P'//RUNFILE(1:RLEN)
c     XFILE='X'//RUNFILE(1:RLEN)
     OAFILE=DFILE(1:DLEN)//'.A'
     OBFILE=DFILE(1:DLEN)//'.B'
     ONFILE=DFILE(1:DLEN)//'.NV'

c  ***** Convert start time   *****

     READ(ATIME,5) TH,TM
 5   FORMAT(2I2.2)
     T0=(TH*60+TM)*60

          chflag=4
          avg=2

          tstart=t0-180
c  ***** Read loss factor data from Ifile *****


     OPEN(10,FILE=IFILE,STATUS='OLD')

       read(10,*)
       read(10,*)

     DO I=1,114
        READ(10,*) D(I),LOSS(I)
     enddo
     CLOSE(UNIT=10)
          do i=1,57
```

```
                d(i)=(d(i)+d(115-i))/2.
                loss(i)=(loss(i)+loss(115-i))/2.
        enddo


c  ***** Create inversion matrix to remove multiply charged peaks *****

    CALL CHRGMAT(CHFLAG,57,D,loss,MCHRG)

c  ***** Open inverted and raw data files and find start time  *****

    DEXT=1
    T=0
    CALL OPENFILE(DIFILE,DEXT,EFLAG,dlen)
 7   READ(12,10,END=800) adum,timsec,dum1,dum2,cb(1),dum3,ca(1)
 10  FORMAT(A1,6f10.2,f10.2,f10.2,f10.2)
        if(timsec.lt.tstart)then
                do i=2,114
                        read(12,*,end=800)
                enddo
                goto 7
        endif

        do i=2,114
          read(12,10,end=800) adum,timsec,dum1,dum2,cb(i),dum3,ca(i)
        enddo


c  ***** Read sets of data and times   *****

 17   DO I=1,114
       SUMA(I)=ca(i)
       SUMB(I)=cb(i)
     ENDDO
     DO K=1,AVG-1
       DO I=1,114
             read(12,10,end=800) adum,timsec,dum1,dum2,cb(i),dum3,ca(i)
         SUMA(I)=SUMA(I)+CA(i)
         SUMB(I)=SUMB(I)+CB(i)
       ENDDO
     ENDDO



c  ***** Average sets of up and down scans   *****

     DO I=1,57
       dnA(I)=(SUMA(I)+suma(115-i))/AVG/2.
       dnB(I)=(SUMB(I)+sumb(115-i))/AVG/2.
     ENDDO


c  ** ** **
c  ***** Correct for multiple charging *****

     DO I=1,57
       DNTA(I,T)=0.
```

```
      DNTB(I,T)=0.
      DO J=1,57
        DNTA(I,T)=DNTA(I,T)+DNA(J)*MCHRG(I,J)
        DNTB(I,T)=DNTB(I,T)+DNB(J)*MCHRG(I,J)
      ENDDO
    ENDDO

c  ***** Calculate time *****

    TAVE=(timsec-60*avg)/60.
    TIM(T)=Tave-(t0/60.)
          dt=tim(t)-tim(t-1)

    HR = TAVE/60.
    MIN = TAVE-60.*HR

    WRITE(*,20) HR,MIN
 20  FORMAT('+ Time =',I2':',I2)
    T=T+1

    NTOTA(t)=0.
    VTOTA(T)=0.
    NTOTB(t)=0.
    VTOTB(T)=0.
          satota(t)=0.
          satotb(t)=0.
    NTOTAc(t)=0.
    VTOTAc(T)=0.
    NTOTBc(t)=0.
    VTOTBc(T)=0.
          satotac(t)=0.
          satotbc(t)=0.



    DO I=1,57


          dl=alog10(d(i)/1000.)
          pk=3.54345+13.4646*dl+9.16105*dl**2+1.8378*dl**3
          beta=dt*10.**pk

      if(i.eq.1)then
        DL=alog(D(i+1)/D(i))
      elseif(i.eq.57)then
        DL=alog(D(i)/D(i-1))
      else
        DL=alog(D(i+1)/D(i-1))/2.
      endif


           na=DNTA(i,t)*DL
      ntota(t)=ntota(t)+na
      va=DNTA(i,t)*DL*3.1416/6.*D(i)**3.*1e-9
      vtota(t)=vtota(t)+va
```

```
            sa=dnta(i,t)*dl*3.1416*d(i)**2.*1e-6
            satota(t)=satota(t)+sa

            nlossa=beta*na + nlossa
            vlossa=beta*va + vlossa
            salossa=beta*sa + salossa

            nb=DNTB(i,t)*DL
          ntotb(t)=ntotb(t)+nb
          vb=DNTB(i,t)*DL*3.1416/6.*D(i)**3.*1e-9
          vtotb(t)=vtotb(t)+vb
            sb=dntb(i,t)*dl*3.1416*d(i)**2.*1e-6
            satotb(t)=satotb(t)+sb

            nlossb=beta*nb + nlossb
            vlossb=beta*vb + vlossb
            salossb=beta*sb + salossb


        ENDDO

           ntotac(t) = ntota(t) + nlossa
           vtotac(t)=vtota(t)+vlossa
           satotac(t)=satota(t)+salossa
            ntotbc(t)=ntotb(t)+nlossb
           vtotbc(t)=vtotb(t)+vlossb
           satotbc(t)=satotb(t)+salossb


c  ***** Go back and read another set of scans  *****

        GOTO 7

c  ***** Open next in series of inverted and raw data files *****

 800  DEXT=DEXT+1
        CALL OPENFILE(DIFILE,DEXT,EFLAG,dlen)
        IF(EFLAG.EQ.-1)THEN
          GOTO 27
        ELSE
          GOTO 7
        ENDIF

c  ***** Write to output files   *****

c     ***   Averaged files ***

 27   OPEN(14,FILE=OAFILE)
        WRITE(14,30) (TIM(TT),TT=1,T)
 30   FORMAT('    Dp(nm)   ',120(I3,9X))
        DO I=1,57
          WRITE(14,40) D(I),(DNTA(I,TT),TT=1,T)
 40       FORMAT(1X,F8.2,4X,120(1PG12.4))
        ENDDO
        CLOSE(14)

        OPEN(14,FILE=OBFILE)
```

```
      WRITE(14,30) (TIM(TT),TT=1,T)
      DO I=1,57
        WRITE(14,40) D(I),(DNTB(I,TT),TT=1,T)
      ENDDO
      CLOSE(14)

      OPEN(14,FILE=ONFILE)
      WRITE(14,50)
 50   FORMAT(' Time(min)      NA        VA        SA',
     &     '        NAcorr     VAcorr     SAcorr',
     &     '    NB        VB        SB',
     &     '        NBcorr     VBcorr     SBcorr')

      DO I=1,T
          WRITE(14,60) TIM(I),NTOTA(I),VTOTA(I),SATOTA(I),
     &               NTOTAc(I),VTOTAc(I),SATOTAc(I),
     &               NTOTB(I),VTOTB(I),SATOTB(I),
     &               NTOTBc(I),VTOTBc(I),SATOTBc(I)
 60     FORMAT(1X,I3,9X,12(1PG12.4))
      ENDDO
      CLOSE(14)

 999  STOP
      END



C**********************************************************************
C**********************************************************************

      SUBROUTINE CHRGMAT(FLAG,N,D,RF,MCHRG)

C     *****   Subroutine to create inversion matrix for removing      *****
C     *****   multiply charged peaks from DMA data                    *****

      real d(120),F1A(100),F1(100),f1b(100),f2b(100)
      real f1c(100),f2c(100),f3c(100),f4c(100),RF(120)
      real z1(100),z2(100),z3(100),z4(100),m(100,100)
      REAL mCHRG(100,100),b(10,10),A(10,10)
      real dl(100)

      do i=1,N


        if(i.eq.1)then
          dl(i)=alog(d(i+1)/d(i))
        elseif(i.eq.N)then
          dl(i)=alog(d(i)/d(i-1))
        else
          dl(i)=alog(d(i+1)/d(i-1))/2
        endif
      enddo

C     *****   Old Fuchs distribution     *****

      a(1,1)=-2.774
      a(1,2)=1.368
```

```
      a(1,3)=0.4456
      a(1,4)=-0.4483
      a(1,5)=0.06627

C     *****  Wiedensohler approximation of Fuchs distribution  *****
C     *****  {J. Aerosol Sci. (1988) 19, 387}                 *****

      b(1,1)=-2.3484
      b(1,2)=0.6044
      b(1,3)=0.4800
      b(1,4)=0.0013
      b(1,5)=-0.1553
      b(1,6)=0.0320
      b(2,1)=-44.4756
      b(2,2)=79.3772
      b(2,3)=-62.8900
      b(2,4)=26.4492
      b(2,5)=-5.7480
      b(2,6)=0.5049

C     *****  Parameters for Gunn Equation {found in Wiedensohler}  *****

      Cx=0.11
      Cy=log(0.875)
      cx1=0.07


      do i=1,N
        sum1b=0
        sum2b=0
        sum1a=0
        do j=1,5
          sum1a=sum1a+a(1,j)*(alog10(d(i)))**(j-1)
        enddo
        do j=1,6
          sum1b=sum1b+b(1,j)*(alog10(d(i)))**(j-1)
          sum2b=sum2b+b(2,j)*(alog10(d(i)))**(j-1)
        enddo
        f1a(i)=10**sum1a
        f1b(i)=10**sum1b
        f2b(i)=10**sum2b
        f1c(i)=1/Cx1/(2*3.1416*d(i))**0.5*
     &         exp(-((1-Cx1**2*d(i)*(Cy))**2/(2*Cx1**2*d(i))))
        f2c(i)=1/Cx/(2*3.1416*d(i))**0.5*
     &         exp(-((2-Cx**2*d(i)*(Cy))**2/(2*Cx**2*d(i))))
        f3c(i)=1/Cx/(2*3.1416*d(i))**0.5*
     &         exp(-((3-Cx**2*d(i)*(Cy))**2/(2*Cx**2*d(i))))
        f4c(i)=1/Cx/(2*3.1416*d(i))**0.5*
     &         exp(-((4-Cx**2*d(i)*(Cy))**2/(2*Cx**2*d(i))))
      enddo

      do i=1,N
        c=1.+130./d(i)*(1.257+0.4*exp(-1.1*d(i)/130.))
        z1(i)=1.*c/d(i)
        z2(i)=2.*c/d(i)
        z3(i)=3.*c/d(i)
        z4(i)=4.*c/d(i)
```

```
      enddo

c     IF(FLAG2.EQ.1)THEN
       DO I=1,N
         F1(I)=F1A(I)
       ENDDO
c     ELSE
c       DO I=1,N
c         F1(I)=F1B(I)
c       ENDDO
c     ENDIF

      do j=N,1,-1
        m(j,j)=f1b(j)/f1(j)
        IF(FLAG.GE.2)THEN
        k=j
        do i=k,1,-1
          if(z2(j).lt.z1(i))then
            x=(z2(j)-z1(i+1))/(z1(i)-z1(i+1))
            m(i,j)=x*f2b(j)*RF(j)/f1(i)/RF(i)*dl(j)/dl(i)+m(i,j)
            m(i+1,j)=(1-x)*f2b(j)*RF(j)/f1(i+1)/RF(i+1)*
     &              dl(j)/dl(i+1)+m(i+1,j)
            k=i
            goto 7
          endif
        enddo
7       ENDIF
        IF(FLAG.GE.3)THEN
        do i=k,1,-1
          if(z3(j).lt.z1(i))then
            x=(z3(j)-z1(i+1))/(z1(i)-z1(i+1))
            m(i,j)=x*f3c(j)*RF(j)/f1(i)/RF(i)*dl(j)/dl(i)+m(i,j)
            m(i+1,j)=(1-x)*f3c(j)*RF(j)/f1(i+1)/RF(i+1)*
     &              dl(j)/dl(i+1)+m(i+1,j)
            k=i
            goto 8
          endif
        enddo
8       ENDIF
        IF(FLAG.GE.4)THEN
        do i=k,1,-1
          if(z4(j).lt.z1(i))then
            x=(z4(j)-z1(i+1))/(z1(i)-z1(i+1))
            m(i,j)=x*f4c(j)*RF(j)/f1(i)/RF(i)*dl(j)/dl(i)+m(i,j)
            m(i+1,j)=(1-x)*f4c(j)*RF(j)/f1(i+1)/RF(i+1)*
     &              dl(j)/dl(i+1)+m(i+1,j)
            k=i
            goto 9
          endif
        enddo
9       ENDIF
      enddo

      call gj(M,N,MCHRG)

      OPEN(UNIT=20,FILE='M')
```

```
      DO I=1,N
        WRITE(20,79) (MCHRG(I,J),J=1,N)
 79     FORMAT(100F8.3)
      ENDDO


      RETURN
      END

C*************************************************************************C*************
************************************************************

      SUBROUTINE OPENFILE(DIFILE,DEXT,EFLAG,dlen)

      CHARACTER*8 DIFILE,DRFILE,IFILE,RFILE
      CHARACTER*1 EXT(8)
      CHARACTER*80 DUM
      INTEGER EFLAG,DEXT,dlen,dl
      REAL TSTART

      DATA EXT/'a', 'b', 'c', 'd', 'e', 'f', 'g', 'h'/

c     EXT=DEXT+64
      dl=dlen
      IFILE=DIFILE(1:dl)//EXT(DEXT)

      write(*,*) 'about to open data file...', ifile

c     RFILE=DRFILE(1:dl)//EXT
      OPEN(12,FILE=IFILE,STATUS='OLD',ERR=17)
c     OPEN(13,FILE=RFILE,STATUS='OLD',ERR=17)
      WRITE(*,10) IFILE,RFILE
 10   FORMAT(' Reading from files: ',a8,4x,a8,/)


      DO I=1,18
        READ(12,30) DUM
 30     FORMAT(A80)
      ENDDO


      GOTO 999
 17   EFLAG=-1

 999  RETURN
      END

C*************************************************************************C*************
************************************************************


      SUBROUTINE GJ(A,N,B)

!     Subroutine performs Gauss-Jordan reduction to invert the matrix A.
!     Taken from Numerical Recipes.
!
!
```

```
!     A = N x N matrix, must be nonsingular
!     B = inverse of A, returned to program
!

      REAL A(100,100),AA(100,100),b(100,100)
      REAL BIG,DUM,PIVINV
      INTEGER IPIV(100),IROW,ICOL

      do i=1,n
        do j=1,n
          aa(i,j)=a(i,j)
          b(i,j)=0.0
        enddo
        b(i,i)=1
      enddo

      DO 100 J=1,N
        IPIV(J)=0
100   CONTINUE
      DO 200 I=1,N
        BIG=0.0
        DO 210 J=1,N
          IF(IPIV(J).NE.1)THEN
            DO 220 K=1,N
              IF(IPIV(K).EQ.0)THEN
                IF(ABS(AA(J,K)).GE.BIG)THEN
                  BIG=ABS(AA(J,K))
                  IROW=J
                  ICOL=K
                ENDIF
              ELSEIF(IPIV(K).GT.1)THEN
                WRITE(5,*) ' * SINGULAR'
                GOTO 999
              ENDIF
220           CONTINUE
          ENDIF
210       CONTINUE
        IPIV(ICOL)=IPIV(ICOL)+1
        IF(IROW.NE.ICOL)THEN
          DO 230 L=1,N
            DUM=AA(IROW,L)
            AA(IROW,L)=AA(ICOL,L)
            AA(ICOL,L)=DUM
230         CONTINUE

        do 240 l=1,N
          dum=b(irow,l)
          b(irow,l)=b(icol,l)
          b(icol,l)=dum
240       continue

        ENDIF
        IF(AA(ICOL,ICOL).EQ.0)THEN
          WRITE(5,*) ' SINGULAR'
          GOTO 999
        ENDIF
        PIVINV=1/AA(ICOL,ICOL)
```

```
      DO 250 L=1,N
        AA(ICOL,L)=AA(ICOL,L)*PIVINV
250   CONTINUE
      DO 260 L=1,N
        B(ICOL,L)=B(ICOL,L)*PIVINV
260   CONTINUE
      DO 270 LL=1,N
        IF(LL.NE.ICOL)THEN
          DUM=AA(LL,ICOL)
          DO 280 L=1,N
            AA(LL,L)=AA(LL,L)-AA(ICOL,L)*DUM
280       CONTINUE
          do 290 l=1,N
            b(ll,l)=b(ll,l)-b(icol,l)*dum
290       continue
        ENDIF
270   CONTINUE
200 CONTINUE

999 RETURN
    END

C**********************************************************************
```

Additional file used in above code to correct for particle losses in DMA:

loss.tbl

Dp [nm]	F
11.95	0.0491
12.52	0.0665
13.11	0.0886
13.74	0.1150
14.39	0.1440
15.08	0.1752
15.79	0.2085
16.56	0.2428
17.35	0.2782
18.18	0.3129
19.05	0.3450
19.97	0.3731
20.93	0.4034
21.94	0.4375
23.00	0.4717
24.11	0.5035
25.28	0.5325
26.50	0.5556
27.79	0.5741
29.14	0.5956
30.57	0.6171
32.07	0.6406
33.64	0.6659
35.29	0.6871
37.03	0.7025
38.87	0.7165
40.79	0.7323
42.82	0.7483
44.96	0.7653
47.21	0.7828
49.59	0.7983
52.09	0.8127
54.72	0.8219
57.51	0.8265
60.45	0.8318
63.56	0.8390
66.84	0.8475
70.30	0.8585
73.97	0.8711
77.85	0.8842
81.96	0.8980
86.31	0.9058
90.92	0.9100
95.82	0.9137
101.01	0.9163
106.53	0.9179
112.40	0.9189

118.65	0.9193
125.30	0.9198
132.39	0.9201
139.96	0.9206
148.04	0.9210
156.68	0.9214
165.92	0.9217
175.82	0.9219
186.44	0.9220
197.83	0.9221
199.18	0.9221
187.69	0.9220
176.98	0.9219
167.01	0.9217
157.69	0.9214
148.99	0.9211
140.85	0.9206
133.23	0.9202
126.08	0.9198
119.38	0.9194
113.09	0.9189
107.18	0.9181
101.62	0.9165
96.39	0.9141
91.46	0.9103
86.82	0.9065
82.44	0.8991
78.30	0.8858
74.40	0.8725
70.71	0.8598
67.22	0.8486
63.92	0.8398
60.80	0.8326
57.83	0.8268
55.03	0.8226
52.38	0.8141
49.86	0.8000
47.48	0.7846
45.21	0.7673
43.06	0.7501
41.02	0.7340
39.08	0.7183
37.24	0.7039
35.49	0.6890
33.82	0.6689
32.24	0.6434
30.74	0.6196
29.30	0.5980
27.94	0.5765
26.64	0.5579
25.41	0.5353
24.24	0.5070
23.12	0.4754
22.06	0.4415
21.04	0.4072
20.08	0.3760
19.15	0.3484
18.28	0.3167
17.44	0.2822
16.65	0.2468
15.88	0.2123
15.16	0.1789
14.47	0.1474
13.81	0.1182
13.18	0.0915
12.59	0.0687
12.02	0.0509

APPENDIX B

Hydrocarbon Measurements and Particle Number, Volume and Surface Area Concentrations for 1994 Aromatic Experiments

Table B.1. Hydrocarbon data for aerosol yield measurements.

EXPERIMENT 8/19/94

SIDE A		SIDE B	
time	toluene	time	*m*-xylene
min	ppb	min	ppb
0	163	0	833
57	162	11	624
101	162	42	719
146	159	71	549
176	160	101	430
146	159	161	240
176	157	193	216
206	153	220	194
236	154	251	140
267	151	282	127
297	149	312	111
327	147	341	112
355	146	371	88
387	145	401	86
417	142	432	80
446	141	459	73

EXPERIMENT 8/21/94

SIDE A			SIDE B		
time	*m*-xylene	propene	time	*p*-xylene	propene
min	ppb	ppb	min	ppb	ppb
0	651	99	0	471	156
10	589	118	24	423	119
37	538	95	51	432	73
65	474	83	80	423	97
95	375	74	113	432	87
98	324	44	142	383	78
128	253	55	172	286	92

157	198	8	204	319	80
187	158	56	233	257	54
219	171	29	263	228	65
248	130	23	293	167	21
278	108	-	322	141	31
307	109	36			
337	102	79			

EXPERIMENT 8/23/94

SIDE A			SIDE B		
time	toluene	propene	time	*p*-xylene	propene
min	ppb	ppb	min	ppb	ppb
0	676	-	0	442	105
8	676	-	23	423	90
37	641	-	52	459	108
67	655	-	81	430	95
96	668	-	111	434	75
126	648	-	140	416	65
155	614	-	170	427	92
185	627	-	200	374	61
214	657	-	235	390	348
250	639	-	264	363	50
279	638	-	296	349	66
309	602	-	323	331	41
338	640	-	353	310	55
367	605	-	382	291	16
396	608	-	419	285	6
426	572	-	440	269	32
455	562	-	473	272	46
488	559	-	502	264	52
517	555	-	531	268	20

EXPERIMENT 8/25/94

SIDE A			SIDE B		
time	propene	ethylbenzene	time	propene	toluene
min	ppb	ppb	min	ppb	ppb
0	112	468	0	139	377
			13	138	381
			23	89	378
38	111	444	52	97	362
67	70	426	81	69	370
96	111	442	111	72	353
125	96	441	140	75	373

154	94	417	170	85	340
185	82	413	199	72	363
214	59	384	228	38	326
243	39	382	257	52	325
272	63	381	286	23	299
301	71	369	315	19	305
338	33	353	353	25	295
367	59	349	382	20	295
396	42	337	411	4	267
425	66	338	440	19	268
455	30	313	469	22	259
484	60	316	499	17	260
513	82	327	527	33	239
542	88	309			

EXPERIMENT 8/27/94

SIDE A

time	ethylbenzene	propene	time	propene	1,2,4-trimethylbenzene
min	ppb	ppb	min	ppb	ppb
0	168	226	0	214	215
11	172	228	26	213	215
42	174	231	56	193	188
70	173	215	84	143	146
99	157	188	115	75	110
130	167	171	145	34	68
161	170	160	176	65	47
191	157	143	206	20	34
220	155	151	235	70	27
249	147	153	264	51	28
278	134	151	293	65	23
308	136	76	324	29	17
339	136	133	355	61	17
370	134	74	385	60	17
401	127	135			

EXPERIMENT 8/29/94

SIDE A

time	propene	ethylbenzene	time	propene	*p*-ethyltoluene
min	ppb	ppb	min	ppb	ppb
0	240	252	0	250	223
14	231	252	29	235	235
44	220	268	60	242	246

75	200	255	90	230	227
106	206	251	120	212	234
135	191	270	149	206	223
164	183	262	179	184	211
193	177	259	208	171	204
224	171	255	239	161	193
254	184	261	270	149	180
285	161	251	300	123	149
315	149	251	331	152	143
346	121	231	361	117	115
376	126	231	407	101	95
392	130	223	438	131	85
422	109	229	468	103	86
453	110	218			

EXPERIMENT 9/2/94

SIDE A			SIDE B		
time	propene	*p*-ethyltoluene	time	propene	toluene
min	ppb	ppb	min	ppb	ppb
0	212	270	0	186	558
6	185	265	27	147	533
41	167	252	56	120	546
70	160	257	85	104	537
100	144	247	115	118	504
129	137	247	144	83	476
160	121	234	176	89	539
192	67	208	208	67	480
223	44	213	237	14	475
251	5	193	265	43	449
279	-12	173	293	-20	452
308	-22	172	322	-7	418
336	21	166	352	-28	420
368	-55	147	384	-39	415

EXPERIMENT 9/4/94

SIDE A			SIDE B		
time	propene	*m*-xylene	time	propene	1,2,4-trimethylbenzene
min	ppb	ppb	min	ppb	ppb
0	190	562	0	201	304
13	132	568	28	183	317
42	74	514	57	127	262
72	48	467	86	75	221

101	-24	421	115	53	190
130	-71	379	145	-6	169
159	-66	363	177	-26	151
192	-62	350	207	23	143
222	-59	337	237	19	135
252	-62	327	267	-85	132
282	-123	325	270		

EXPERIMENT 9/6/94

SIDE A			SIDE B		
time	propene	*m*-ethyltoluene	time	propene	ethylbenzene
min	ppb	ppb	min	ppb	ppb
0	196	258	0	175	382
11	182	219	25	177	373
40	163	232	55	173	381
70	149	203	85	158	352
99	119	163	114	147	365
129	76	131	144	148	357
158	89	109	173	145	352
187	47	90	202	123	332
217	65	77	232	111	338
246	48	75	261	74	323
276	95	72	291	69	320
336	62	61	321	93	309
367	58	60	352	94	300
397	83	59	382	103	293
428	88	55	412	88	288
458	85	57	443	70	253
489	85	55	474	107	272
			504	95	264

EXPERIMENT 9/8/94

SIDE A			SIDE B		
time	propene	*p*-xylene	time	propene	1,2,4-trimethylbenzene
min	ppb	ppb	min	ppb	ppb
0	221	1084	0	193	335
29	224	1076	13	260	321
59	222	1073	44	273	275
88	231	1061	73	220	254
118	196	1026	103	212	182
148	168	995	133	135	163

178	185	970	163	178	122
207	136	922	193	184	106
237	143	868	222	171	110
267	120	819	252	188	93
296	145	805	282	182	87
326	140	765	311	203	87
356	159	760	341	229	83

EXPERIMENT 9/10/94

SIDE A			SIDE B		
time	propene	*p*-ethyltoluene	time	propene	*m*-ethyltoluene
min	ppb	ppb	min	ppb	ppb
0	213	365	0	219	220
13	195	422	28	193	218
43	185	387	59	177	212
74	180	407	89	132	182
104	167	383	119	95	157
133	150	354	148	53	134
163	127	352	178	84	121
192	91	316	207	61	107
222	117	321	237	48	99
252	87	281	267	78	93
282	83	272	297	74	93
312	52	247	327	24	85
342	60	236	357	72	86

EXPERIMENT 9/12/94

SIDE A			SIDE B		
time	propene	*p*-xylene	time	propene	ethylbenzene
min	ppb	ppb	min	ppb	ppb
0	140	421	0	138	329
0	119	407	0	118	322
0	120	415	2	122	319
17	143	404	32	141	319
46	111	400	61	127	324
76	119	395	91	127	326
106	119	384	121	105	324
136	107	386	151	95	309
166	79	374	181	99	292
196	68	359	211	88	283
226	67	344	241	60	291

256	55	335	271	62	275
257	48	334	301	68	292
286	27	309	332	76	274
286	32	307	361	55	279
317	17	302	391	73	276
316	38	296	421	71	279

EXPERIMENT 9/14/94

SIDE A			SIDE B		
time	propene	*m*-xylene	time	propene	ethylbenzene
min	ppb	ppb	min	ppb	ppb
0	158	380	0	157	249
13	160	391	28	152	241
43	151	376	58	128	207
73	155	371	88	117	145
104	147	387	119	102	130
134	142	362	149	88	86
163	135	346	179	87	86
194	146	343	209	82	66
224	129	346	238	83	70
253	135	333	268	76	54
283	119	312	298	83	55
313	110	310	327	71	49
312	91	291	357	89	52
343	101	262	387	85	46
342	76	255	417	77	47

EXPERIMENT 9/16/94

SIDE A			SIDE B		
time	propene	toluene	time	propene	1,2,4-trimethylbenzene
min	ppb	ppb	min	ppb	ppb
0	215	500	0	210	249
13	216	495	28	234	276
43	197	488	58	195	254
73	207	495	87	203	221
102	172	488	117	176	178
131	188	485	146	177	149
161	170	484	175	156	132
190	165	483	205	138	124
219	165	480	234	126	114
249	160	469	264	139	115
279	137	473	294	144	110

309	132	465	324	120	106
309	135	463	354	125	105
339	117	461	385	130	105

EXPERIMENT 9/19/94

SIDE A			SIDE B		
time	propene	toluene	time	propene	*m*-ethyltoluene
min	ppb	ppb	min	ppb	ppb
0	26	423	0	45	451
0	-11	427	12	40	418
26	-10	425	41	52	396
55	-1	426	69	-2	368
84	-5	419	98	-27	328
113	-7	423	127	-17	293
142	-35	419	157	-101	267
173	-29	421	188	-110	228
204	-24	405	219	-140	213
235	-96	408	250	-127	200
265	-54	403	281	-132	201
296	-73	400	312	-140	194

EXPERIMENT 9/21/94

SIDE A			SIDE B		
time	propene	*p*-xylene	time	propene	1,2,4-trimethylbenzene
min	ppb	ppb	min	ppb	ppb
0	266	543	0	269	202
14	299	547	29	292	244
44	283	548	59	253	177
73	262	551	89	255	169
103	247	545	118	218	132
133	226	540	148	195	111
162	202	537	177	191	94
191	233	532	207	141	87
221	182	529	236	147	73
251	210	521	266	128	70
280	183	517	296	158	66
310	150	510	325	165	64
340	152	509	354	147	63
369	134	504	384	157	63

EXPERIMENT 9/30/94

SIDE A			SIDE B		
time	propene	toluene	time	propene	toluene
min	ppb	ppb	min	ppb	ppb
0	17	316	0	160	297
0	5	32	0	137	292
30	-	308	30	134	293
59	-	317	59	115	303
89	-	309	89	119	294
119	-	314	119	101	290
149	-	309	149	110	274
179	-	295	179	81	274
209	-	302	209	90	257
239	-	295	239	82	256
269	-	301	269	66	246
299	13	282	300	53	242
329	33	278	330	69	236
360	34	282	360	60	221
390	36	267	390	63	216
412	44	266			

EXPERIMENT 10/6/94

SIDE A			SIDE B		
time	propene	*m*-ethyltoluene	time	propene	1,2,4-trimethylbenzene
min	ppb	ppb	min	ppb	ppb
0	184	193	0	168	437
30	158	177	30	178	438
61	158	168	61	144	430
91	140	173	91	163	430
122	142	148	182	96	363
212	98	96	212	106	360
241	82	91	241	92	341
271	98	73	271	85	331
301	72	63	301	64	324
331	81	59	331	74	321
361	74	49	359	64	319

EXPERIMENT 10/10/94

SIDE A			SIDE B		
time	propene	toluene	time	propene	*p*-ethyltoluene
min	ppb	ppb	min	ppb	ppb
0	230	223	0	205	279
30	196	212	30	223	273

59	192	205	60	224	250
89	186	198	90	194	272
119	177	213	120	193	273
150	205	190	150	179	251
180	164	190	180	197	257
210	132	183	210	179	220
240	137	177	240	181	225
270	129	174	270	150	200
300	126	163	300	113	207
329	160	164	330	119	177
359	153	154	359	151	178
389	102	152	389	125	166
419	144	144	419	142	163
449	132	143	449	117	157
479	94	136	479	148	163

EXPERIMENT 10/16/94

SIDE A			SIDE B		
time	propene	1,2,4-trimethyl-benzene	time	propene	1,2,4-trimethylbenzene
min	ppb	ppb	min	ppb	ppb
0	329	501	0	267	504
13	280	514	28	249	414
42	282	503	56	247	386
71	284	447	86	227	417
101	280	392	116	204	359
130	219	316	145	175	319
160	204	279	175	142	251
190	171	276	206	120	227
221	154	245	236	100	228
252	138	212	267	94	201
282	130	203	298	103	189

EXPERIMENT 10/18/94

SIDE A			SIDE B		
time	propene	*p*-ethyltoluene	time	propene	1,2,4-trimethylbenzene
min	ppb	ppb	min	ppb	ppb
0	339	313	0	285	6901
13	310	272	28	301	5776
42	318	301	57	272	6117
72	295	275	87	257	6306
101	294	266	116	259	4370
131	312	265	147	210	3211

162	291	244	177	183	2461
192	282	259	207	187	1865
222	251	236	237	182	1190
253	301	252	268	141	968
283	258	209	298	145	651
313	285	189	328	123	561
343	232	202	358	136	519

EXPERIMENT 10/20/94

SIDE A			SIDE B		
time	propene	*m*-xylene	time	propene	*m*-ethyltoluene
min	ppb	ppb	min	ppb	ppb
0	295	377	0	284	165
0	279	401	0	297	209
0	277	386	0	268	187
14	274	396	29	261	214
44	240	372	59	244	172
74	242	345	89	245	164
104	229	296	119	243	142
134	196	261	149	221	125
164	163	226	180	178	102
195	143	193	210	190	105
225	155	158	240	157	77
255	147	148	270	168	73

EXPERIMENT 10/22/94

SIDE A			SIDE B		
time	propene	*m*-ethyltoluene	time	propene	*p*-xylene
min	ppb	ppb	min	ppb	ppb
0	84	256	0	95	6504
0	78	252	0	71	6243
13	75	248	27	82	6662
42	85	253	57	76	6164
72	72	236	86	68	6439
101	63	196	116	74	6261
131	52	187	147	62	6009
162	45	176	177	68	5634
192	52	167	208	52	5712
223	8	146	238	44	5480
254	20	138	269	60	5682
284	4	125	299	47	5469
314	-14	127	329	46	5319

344	-41	100	359	61	4969
374	-7	102	380	49	4999

EXPERIMENT 10/30/94

SIDE A			SIDE B		
time	propene	*p*-ethyltoluene	time	propene	1,2,4-trimethylbenzene
min	ppb	ppb	min	ppb	ppb
0	188	301	0	179	6758
13	166	298	28	171	6343
43	164	305	59	162	5142
73	162	279	88	146	5214
103	147	283	118	122	4176
133	158	300	148	121	3515
162	142	286	177	105	2416
192	139	278	207	99	1986
223	144	266	238	85	1502
253	137	243	268	83	1212
283	133	247	298	78	1159
313	144	245	328	70	1125

EXPERIMENT 11/1/94

SIDE A			SIDE B		
time	propene	*p*-ethyltoluene	time	propene	*p*-xylene
min	ppb	ppb	min	ppb	ppb
0	451	271	0	416	611
14	436	261	29	393	610
44	423	269	59	371	616
74	402	257	89	351	532
104	394	257	119	346	604
134	399	241	149	341	487
164	407	241	179	318	510
194	360	225	209	302	390
224	356	229	238	303	403
253	332	235	268	298	363
283	325	201	297	260	369
312	341	198	327	294	287
342	321	188	357	269	269
372	303	181	387	244	264

EXPERIMENT 11/4/94

SIDE A			SIDE B		
time	propene	*m*-ethyltoluene	time	propene	*p*-xylene
min	ppb	ppb	min	ppb	ppb
0	161	406	0	140	573
13	191	433	28	146	605
42	168	434	57	143	589
72	176	392	87	130	582
102	155	408	117	131	557
132	138	374	147	119	578
162	122	285	177	123	541
192	93	226	208	115	557
223	76	208	238	97	551
253	56	194	269	89	535
284	36	188	299	94	499
314	37	148	328	92	501
343	38	149	358	79	507

EXPERIMENT 11/9/94

SIDE A			SIDE B		
time	propene	*p*-ethyltoluene	time	propene	*m*-xylene
min	ppb	ppb	min	ppb	ppb
0	211	336	0	174	900
12	207	377	0	161	901
42	182	388	27	143	789
71	155	372	57	143	831
101	157	362	86	122	726
131	189	368	116	111	635
161	207	352	146	119	527
192	166	321	176	66	394
222	161	340	207	37	309
252	156	313	237	20	295
282	172	306	267	34	219
312	140	329	297	-13	219
342	130	279	327	13	185
373	101	296	358	10	211

Table B.2. Time-dependent aerosol particle concentrations, volume concentrations, and surface area concentrations for toluene 1994 experiments.

NA, NB = particle number concentration not corrected for particle losses to walls (cm^{-3})
VA, VB = volume concentration not corrected for particle losses ($\mu m^3\ cm^{-3}$)
SA, SB = surface area concentration not corrected for particle losses ($\mu m^2\ cm^{-3}$)

NAcorr, NBcorr = particle number concentration corrected for particle losses (cm^{-3})
VAcorr, VBcorr = volume concentration corrected for particle losses ($\mu m^3\ cm^{-3}$)
SAcorr, SBcorr = surface area concentration corrected for particle losses ($\mu m^2\ cm^{-3}$)

8/19/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
0	1108	0.8261	36.81	1108	0.8261	36.81
5	629.3	0.1193	8.256	641	0.1215	8.392
9	650.6	0.1263	8.659	671.8	0.1303	8.909
14	631.2	0.1191	8.271	664.2	0.1251	8.655
18	620.6	0.1189	8.284	662.8	0.1266	8.774
23	618.8	0.1206	8.382	672.1	0.1303	9.005
27	595.1	0.1118	7.862	657.3	0.123	8.584
32	601.8	0.1119	7.882	674.9	0.125	8.73
36	577.6	0.1175	7.962	659.5	0.1323	8.913
40	591.8	0.1217	8.16	682.4	0.1382	9.218
45	590.5	0.1179	8.026	692.1	0.1365	9.216
49	561.8	0.114	7.821	671.6	0.1343	9.111
54	570.3	0.1098	7.679	690.1	0.1319	9.09
58	566.3	0.1134	7.75	694.2	0.1372	9.264
63	573	0.1092	7.624	711.3	0.1348	9.258
67	553.1	0.1059	7.426	699.4	0.1329	9.154
73	558.1	0.1069	7.567	716.4	0.136	9.436
77	545.8	0.1097	7.548	711.9	0.1403	9.514
82	545.3	0.1089	7.57	721.1	0.1413	9.652
86	539.9	0.1086	7.435	723.5	0.1425	9.613
90	538.8	0.1061	7.434	730.1	0.1413	9.703
95	511.8	0.1074	7.313	712.1	0.1444	9.696
99	503	0.1035	7.091	710.2	0.142	9.564
104	513.6	0.1014	7.112	729.7	0.1416	9.696
108	526.3	0.1145	7.748	749.5	0.1562	10.43
113	532.1	0.1114	7.611	764.6	0.1549	10.41
117	520.1	0.1126	7.665	759.6	0.1577	10.56
122	510	0.1132	7.599	758.2	0.1603	10.62
126	522.6	0.1208	8.015	777.7	0.1696	11.13
131	511.8	0.1171	7.776	775.5	0.1678	11.02
135	521.9	0.1277	8.329	792.5	0.1802	11.68

140	509.7	0.1307	8.312	788.8	0.1856	11.79
144	509.2	0.1264	8.192	794.9	0.1831	11.78
148	499.5	0.1344	8.549	791.6	0.1929	12.24
153	505.6	0.1506	9.092	805.8	0.212	12.94
157	511.4	0.1421	8.934	818	0.2056	12.9
162	503.9	0.1405	8.886	818.4	0.2063	12.99
166	477.5	0.1317	8.372	797.9	0.1994	12.58
171	483.4	0.1433	8.911	811.1	0.2135	13.26
175	493.5	0.1547	9.332	827.3	0.2272	13.8
179	488	0.1511	9.368	827.7	0.2257	13.96
187	585.6	0.1814	11.28	939.1	0.261	16.15
191	720.1	0.2477	14.78	1082	0.331	19.84
196	684.7	0.2354	14.27	1057	0.3228	19.56
200	673.1	0.2449	14.56	1053	0.3357	20.03
205	696.8	0.2551	15.21	1086	0.3504	20.92
209	688.5	0.257	15.36	1086	0.3558	21.26
214	661.5	0.2657	15.46	1068	0.3694	21.61
218	672.6	0.2953	16.83	1086	0.4031	23.19
222	673.8	0.3022	17.34	1095	0.4143	23.92
227	641.1	0.3105	17.34	1071	0.4283	24.19
231	611.8	0.3153	17.34	1049	0.4377	24.43
236	633.9	0.3474	18.83	1080	0.476	26.22
240	649.7	0.3781	20.26	1103	0.5123	27.91
244	646	0.386	20.71	1106	0.5256	28.63
249	643.7	0.4165	21.75	1113	0.5637	30.03
253	640.9	0.4508	22.96	1118	0.6048	31.55
258	627.4	0.489	24.29	1114	0.6522	33.3
262	688.7	0.5912	28.44	1184	0.764	37.86
266	691.1	0.6347	30.1	1196	0.8176	39.97
271	686.2	0.6819	31.65	1202	0.8788	42.11
275	687.8	0.737	33.4	1214	0.9462	44.38
280	690.5	0.8011	35.47	1229	1.027	47.15
284	666.7	0.8564	36.88	1216	1.098	49.17
289	684.1	0.9586	40.16	1248	1.222	53.32
293	688.3	1.034	42.07	1264	1.317	56
297	697.1	1.125	44.2	1287	1.431	59
302	737.1	1.22	46.81	1348	1.559	62.81
306	785.6	1.288	48.51	1415	1.656	65.56
311	821.5	1.339	49.19	1476	1.746	67.65
315	946.8	1.428	51.95	1626	1.87	71.66
320	1044	1.49	53.59	1756	1.981	74.97
324	1218	1.511	54.58	1962	2.042	77.34
328	1355	1.542	55.99	2132	2.115	80.21
341	1891	1.492	57.94	2798	2.202	86.95
346	2028	1.315	54.23	2984	2.07	84.85
350	2209	1.216	53.88	3206	2.001	85.65
355	2484	1.228	57.43	3538	2.05	90.62
359	2728	1.196	60.2	3829	2.042	94.42

364	3102	1.264	67.12	4267	2.138	102.6
368	3466	1.385	75.82	4687	2.281	112.4
372	3825	1.601	87.02	5106	2.521	124.8
377	4188	1.93	102	5553	2.886	141.6
381	4531	2.232	115.9	5968	3.223	157.1
386	4944	2.576	131.4	6478	3.617	175
390	5196	2.909	145.7	6810	3.995	191.4
395	5090	3.065	149.9	6801	4.215	198.4
399	5276	3.464	165.3	7067	4.673	216.4
403	5526	3.856	181.1	7401	5.133	235.1
408	5651	4.319	197.9	7630	5.694	256.1
412	5778	4.753	214.1	7844	6.217	275.9
417	5878	5.16	228.8	8053	6.748	295.6
421	5988	5.545	243.2	8253	7.242	314.2
426	6021	5.975	257.3	8398	7.823	334.3
430	5975	6.278	266.9	8443	8.256	348.8
435	5919	6.608	277.4	8500	8.759	365.9
439	5898	6.884	285.9	8572	9.182	380
443	5873	7.185	295.7	8639	9.639	395.6
448	5798	7.379	301	8680	10.03	408.4
452	5757	7.546	306.6	8731	10.37	420.1
457	5598	7.666	308.2	8686	10.7	429.5

8/25/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
1	126.2	2.82E-02	1.785	126.7	2.83E-02	1.791
5	143.2	3.34E-02	2.095	146	3.40E-02	2.129
10	144.3	3.43E-02	2.068	150	3.56E-02	2.142
23	122.5	2.56E-02	1.677	134.7	2.82E-02	1.828
32	121.2	2.55E-02	1.663	137.9	2.91E-02	1.87
41	132.5	2.44E-02	1.665	153.8	2.88E-02	1.923
50	186.2	4.08E-02	2.62	214.2	4.66E-02	2.961
63	179.5	3.62E-02	2.413	216.7	4.38E-02	2.86
81	163.8	3.32E-02	2.23	212.9	4.33E-02	2.828
90	161.7	3.62E-02	2.342	216.6	4.78E-02	3.017
102	167.9	3.82E-02	2.419	229.7	5.09E-02	3.17
111	168.6	3.06E-02	2.168	236.3	4.44E-02	2.986
120	169.5	3.36E-02	2.28	242.6	4.85E-02	3.164
133	168.1	3.81E-02	2.446	249.5	5.46E-02	3.432
142	175.8	3.53E-02	2.359	263.2	5.31E-02	3.419
151	183.5	4.14E-02	2.666	277.2	6.06E-02	3.809
160	165.8	3.39E-02	2.267	265.2	5.43E-02	3.481
173	173.2	3.70E-02	2.456	280.6	5.90E-02	3.772
182	166	3.82E-02	2.462	278.8	6.15E-02	3.854
191	152.7	3.84E-02	2.403	270.4	6.31E-02	3.869
200	164.8	4.53E-02	2.796	287.4	7.13E-02	4.342
214	169.6	4.16E-02	2.686	299.7	6.98E-02	4.353

223	169.3	4.66E-02	2.881	304.3	7.63E-02	4.635
232	144.4	4.34E-02	2.607	283.9	7.47E-02	4.444
241	152.6	4.64E-02	2.812	296.5	7.93E-02	4.735
249	143.1	4.90E-02	2.843	290.7	8.35E-02	4.843
263	146.8	4.36E-02	2.724	300.6	8.05E-02	4.853
272	152.8	5.59E-02	3.224	310.8	9.45E-02	5.445
280	141.2	4.65E-02	2.845	302.7	8.65E-02	5.14
289	131.6	4.36E-02	2.714	296.6	8.51E-02	5.09
352	129.1	9.46E-02	4.801	317.4	0.1515	7.939
414	289.5	0.2012	8.273	1104	0.3122	15.31
500	1920	0.6721	40.1	3201	0.9304	54.13
522	2048	1.025	55.25	3481	1.348	72.72

9/2/94

Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
1	1701	0.332	23.28	1707	0.3331	23.35
14	1910	0.396	26.86	2004	0.414	27.99
23	1770	0.3456	23.88	1922	0.374	25.71
32	1697	0.3223	22.42	1908	0.3604	24.89
41	1617	0.2958	20.88	1883	0.343	23.96
50	1620	0.2893	20.59	1939	0.3453	24.26
63	1535	0.2701	19.63	1928	0.3374	24.09
72	1505	0.2606	19	1947	0.3355	24
81	1561	0.288	20.51	2053	0.3708	26.06
94	1501	0.2762	19.74	2063	0.3705	26.08
103	1473	0.2778	19.71	2083	0.3798	26.58
112	1442	0.2557	18.76	2099	0.3652	26.16
121	1414	0.2649	19.04	2115	0.3819	26.96
130	1383	0.2586	18.65	2128	0.3828	27.07
139	1370	0.2643	18.78	2158	0.3959	27.72
152	1319	0.259	18.45	2166	0.4012	28.1
161	1323	0.2581	18.55	2209	0.4076	28.71
170	1290	0.255	18.23	2213	0.4118	28.88
179	1273	0.267	18.67	2233	0.4313	29.81
192	1567	0.3398	23.67	2590	0.5175	35.7
201	1534	0.347	23.99	2599	0.5345	36.66
213	1528	0.3528	24.39	2648	0.5533	37.9
222	1482	0.3556	24.35	2642	0.5661	38.51
231	1481	0.3822	25.7	2679	0.603	40.52
239	1427	0.3892	25.79	2659	0.6196	41.21
248	1453	0.4235	27.71	2720	0.6656	43.83
262	1407	0.4652	29.47	2728	0.7268	46.75
271	1354	0.4732	29.8	2707	0.7477	47.83
279	1384	0.5314	32.58	2766	0.8188	51.35
288	1329	0.5765	34.11	2743	0.8797	53.75
302	1321	0.6395	36.84	2784	0.9698	57.95
311	1301	0.6963	39.11	2795	1.046	61.23
321	1279	0.7722	41.9	2808	1.147	65.28

334	1205	0.8062	42.54	2778	1.216	67.64
343	1195	0.8758	45.02	2798	1.312	71.39
352	1155	0.9288	46.52	2789	1.394	74.25

9/30/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
0	7949	1.337	97	7949	1.337	97
3	7347	1.19	87.11	7436	1.202	87.94
12	6944	1.039	78	7287	1.082	81.11
21	6606	0.9438	72.29	7191	1.015	77.54
30	6502	0.9147	70.7	7323	1.013	77.98
39	6183	0.8741	67.95	7231	0.9973	77.16
54	5973	0.8291	64.69	7384	0.9926	77.02
62	5873	0.8306	64.73	7469	1.015	78.68
71	5704	0.7932	62.43	7502	0.9997	78.13
80	5580	0.7952	62.06	7575	1.024	79.5
89	5379	0.7611	59.79	7564	1.011	78.91
103	5197	0.7462	58.19	7666	1.03	79.89
112	5053	0.749	57.6	7696	1.054	80.92
121	4922	0.7369	56.7	7734	1.063	81.6
129	4837	0.72	55.71	7796	1.064	81.98
143	4611	0.6899	53.53	7813	1.064	82.11
152	4550	0.6945	53.5	7903	1.088	83.56
161	4370	0.6908	52.67	7865	1.103	84.17
171	5548	0.8535	65.81	9244	1.292	99.29
180	5460	0.8614	66.06	9329	1.323	101.3
189	5276	0.847	64.82	9312	1.332	101.8
203	5069	0.8453	64.09	9350	1.366	103.8
211	4964	0.8403	63.56	9380	1.382	104.8
220	4754	0.8383	63.06	9311	1.403	105.9
229	4644	0.8626	63.7	9338	1.451	108.3
243	4503	0.8755	64.71	9393	1.5	111.9
252	4424	0.9202	66.42	9436	1.57	115.3
260	4336	0.9515	67.82	9450	1.624	118.3
269	4244	0.9922	69.77	9467	1.691	122
284	4172	1.077	74.34	9570	1.823	129.6
293	4042	1.121	76.09	9539	1.897	133.3
302	3971	1.205	79.72	9563	2.012	138.9
310	3885	1.265	82.37	9559	2.102	143.3
319	3787	1.405	88.11	9550	2.279	151.2
333	3624	1.536	92.92	9519	2.471	159.6
342	3517	1.641	96.89	9494	2.62	166
350	3406	1.783	101.9	9455	2.805	173.3
359	3830	2.226	123.1	9970	3.309	197.7
373	3539	2.349	125.3	9819	3.536	205.2

Table B.3. Time-dependent aerosol particle concentrations, volume concentrations, and surface area concentrations for ethylbenzene 1994 experiments.

NA, NB = particle number concentration not corrected for particle losses to walls (cm^{-3})
VA, VB = volume concentration not corrected for particle losses ($\mu m^3\ cm^{-3}$)
SA, SB = surface area concentration not corrected for particle losses ($\mu m^2\ cm^{-3}$)

NAcorr, NBcorr = particle number concentration corrected for particle losses (cm^{-3})
VAcorr, VBcorr = volume concentration corrected for particle losses ($\mu m^3\ cm^{-3}$)
SAcorr, SBcorr = surface area concentration corrected for particle losses ($\mu m^2\ cm^{-3}$)

8/25/94						
Time(min)	**NA**	**VA**	**SA**	**NAcorr**	**VAcorr**	**SAcorr**
1	154.1	3.39E-02	2.158	154.7	3.40E-02	2.165
10	163	3.41E-02	2.232	169.3	3.53E-02	2.307
23	331.2	7.93E-02	4.897	348.2	8.38E-02	5.14
32	163.4	5.74E-02	2.879	186.1	6.37E-02	3.209
41	159.8	3.61E-02	2.293	188.1	4.42E-02	2.713
50	155	3.67E-02	2.233	188.6	4.62E-02	2.726
63	147.2	4.71E-02	2.465	188.8	5.97E-02	3.1
72	142.2	3.78E-02	2.205	192.4	5.16E-02	2.911
81	149.2	2.99E-02	1.984	204.4	4.48E-02	2.754
90	151.6	4.37E-02	2.412	212	6.06E-02	3.272
102	138.9	2.88E-02	1.888	237.9	4.68E-02	2.834
111	164.1	2.64E-02	1.878	268.4	4.56E-02	2.888
120	137.1	5.52E-02	2.616	246.1	7.66E-02	3.72
133	139.9	2.83E-02	1.863	258	5.16E-02	3.068
142	211.4	0.2392	9.026	336.3	0.2696	10.51
151	131.2	3.19E-02	1.928	260.3	6.33E-02	3.463
160	122.3	2.94E-02	1.798	271.9	6.19E-02	3.403
173	269.3	2.64E-02	1.925	430.1	6.02E-02	3.617
182	123.3	4.83E-02	2.335	288.3	8.44E-02	4.12
191	116.3	2.77E-02	1.663	291.3	8.08E-02	3.992
200	149.3	2.89E-02	1.731	329.5	8.32E-02	4.122
214	110.2	2.27E-02	1.52	295.5	7.82E-02	3.984
223	107.8	2.73E-02	1.639	296.5	8.38E-02	4.153
232	112	2.12E-02	1.516	304.1	7.87E-02	4.089
241	102.8	3.43E-02	1.857	298.1	9.31E-02	4.49
249	88.13	1.87E-02	1.298	289.2	7.82E-02	3.978
263	103.6	3.09E-02	1.812	313.9	9.27E-02	4.603
272	140.1	0.1126	5.165	354	0.1771	8.079
280	88.02	2.93E-02	1.629	304.2	9.47E-02	4.584
294	80.81	2.70E-02	1.487	313.3	9.74E-02	4.634
303	79.72	2.20E-02	1.328	314.4	9.33E-02	4.518
311	72.11	2.08E-02	1.232	308.7	9.29E-02	4.463

321	76.91	2.44E-02	1.443	331.9	9.78E-02	4.748
330	73.13	2.50E-02	1.475	330	9.93E-02	4.823
343	72.53	2.28E-02	1.396	331.9	9.80E-02	4.799
352	76.75	6.93E-02	2.93	338.1	0.1464	6.41
361	59.92	2.49E-02	1.435	322.6	0.1027	4.954
370	185.3	8.75E-02	3.566	456.2	0.1689	7.221
383	250.8	3.70E-02	2.557	538.8	0.1198	6.299
392	58.83	3.16E-02	1.677	348.2	0.1156	5.469
401	47.07	3.17E-02	1.579	338.5	0.1168	5.427
410	47.45	3.36E-02	1.635	340.1	0.1199	5.536
423	49.91	4.17E-02	1.914	344.6	0.1301	5.909
432	46.37	3.75E-02	1.783	343.1	0.1275	5.848
442	192.3	7.23E-02	4.385	492	0.1648	8.562
451	50.72	4.70E-02	2.119	352.1	0.1412	6.373
460	45.26	4.58E-02	1.981	353.3	0.1421	6.324
473	42.06	4.57E-02	1.881	353.6	0.146	6.392
482	48.15	6.15E-02	2.387	361.8	0.1642	6.988
491	42.18	6.06E-02	2.278	357.9	0.1654	6.958
504	43.78	5.40E-02	2.063	362.3	0.1628	6.89
513	107.6	0.2199	8.039	429.4	0.3344	13.08
522	47.14	5.73E-02	2.201	370.9	0.1748	7.348
526	45.91	5.53E-02	2.125	370.4	0.1742	7.318
531	107.1	5.55E-02	2.162	437.5	0.176	7.42
535	41.39	4.45E-02	1.7	372.5	0.1661	6.996

8/27/94						
Time(min)	**NA**	**VA**	**SA**	**NAcorr**	**VAcorr**	**SAcorr**
0	2115	0.3858	27.05	2115	0.3858	27.05
12	1850	0.3275	22.81	1934	0.3428	23.77
21	1615	0.2878	20.46	1753	0.312	22.02
30	1608	0.2631	19.52	1805	0.2961	21.68
39	1605	0.3935	23.89	1854	0.4368	26.69
53	1492	0.2771	19.02	1813	0.332	22.57
61	1492	0.2826	19.19	1851	0.3444	23.17
70	1655	0.4017	23.58	2074	0.4758	28.24
83	1452	0.2485	17.94	1943	0.3343	23.38
92	342.5	4.76E-02	2.65	870.2	0.1384	8.386
110	413.8	8.89E-02	6.204	999.3	0.1994	12.78
119	2.92E+04	13.81	671.3	3.03E+04	14.19	689.7
128	1281	0.2323	16.66	2910	0.7132	40.62
137	1209	0.2143	15.72	2879	0.7015	40.11
146	1183	0.1989	14.98	2891	0.692	39.8
155	1209	0.2172	15.94	2953	0.7167	41.2
164	1210	0.2173	15.79	2993	0.7232	41.49
174	393.9	0.2232	10.79	2202	0.7382	36.89
183	1028	0.2067	14.68	2865	0.7276	41.19
192	1019	0.2085	14.74	2886	0.7353	41.65

200	954.9	0.2031	14.37	2846	0.735	41.61
209	909.4	0.2004	14.04	2825	0.7379	41.65
222	896.4	0.2229	15.02	2848	0.7753	43.37
231	833.9	0.2113	14.23	2807	0.7697	42.96
240	806.5	0.1985	13.82	2806	0.7625	42.92
253	750	0.2209	14.49	2777	0.7931	44.11
262	700.3	0.2215	14.32	2744	0.7997	44.3
271	677.8	0.2375	14.9	2738	0.8223	45.27
280	624.2	0.2717	15.89	2699	0.8639	46.66
293	635	0.2779	16.32	2732	0.881	47.68
302	304.2	0.1508	8.595	2412	0.7603	40.3
312	231.5	0.1449	7.793	2350	0.7594	39.77
321	591.1	0.3849	20.43	2724	1.01	52.95
330	582.2	0.4192	21.56	2730	1.057	54.67
343	265.7	0.2423	11.4	2431	0.8962	45.27
352	27.6	5.73E-02	2.095	2196	0.7134	36.07
361	5.158	1.70E-04	8.26E-03	2175	0.6579	34.06
374	494.1	0.5503	24.89	2681	1.23	59.91
383	464.3	0.5636	24.84	2667	1.265	60.75
387	657.4	0.7816	33.3	2870	1.496	69.75
392	456	0.6304	26.65	2678	1.359	63.66
396	447.8	0.6394	26.74	2676	1.379	64.22
401	500.8	0.6629	27.84	2739	1.418	65.91

9/6/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
0	1704	0.2696	20.37	1704	0.2696	20.37
13	1621	0.2485	19.12	1700	0.2588	19.9
22	1589	0.24	18.69	1721	0.257	19.98
30	1589	0.2575	19.35	1767	0.281	21.11
39	1524	0.2477	18.64	1752	0.2783	20.92
53	1813	0.2911	22.04	2135	0.3343	25.26
62	1793	0.287	21.83	2174	0.3382	25.65
71	1771	0.2848	21.59	2209	0.3442	26.01
79	1752	0.2726	20.98	2240	0.3388	25.91
91	1698	0.2783	21.13	2258	0.3549	26.83
100	1698	0.2797	21.17	2312	0.3638	27.43
113	1619	0.2663	20.16	2307	0.3613	27.22
122	1562	0.27	20.13	2299	0.3726	27.74
131	1578	0.2801	20.74	2363	0.39	28.88
140	1500	0.2665	19.86	2330	0.3836	28.52
153	1460	0.2659	19.68	2352	0.3933	29.09
162	1438	0.2636	19.5	2373	0.3982	29.43
171	1527	0.3015	21.79	2506	0.4441	32.28
184	1642	0.3297	23.85	2689	0.4857	35.26
193	1622	0.3466	24.65	2712	0.5117	36.68
204	1563	0.3634	25.33	2705	0.5407	38.17

213	1588	0.3911	26.93	2771	0.5789	40.45
222	1624	0.4415	29.43	2847	0.6417	43.69
231	1610	0.4666	30.85	2872	0.6795	45.9
244	1595	0.5682	35.52	2913	0.8042	51.88
253	1555	0.6445	38.64	2910	0.899	56.01
262	1540	0.7598	43.38	2932	1.036	61.89
271	1483	0.874	47.61	2912	1.176	67.41
279	1465	1.018	53.03	2927	1.347	74.13
293	1405	1.31	62.62	2928	1.7	86.54
302	1421	1.565	71.16	2989	2.008	97.35
312	1378	1.88	79.49	3000	2.399	108.8
321	1399	2.182	86.92	3081	2.789	119.7
330	1444	2.43	92.33	3195	3.149	129.3
339	1623	2.725	99.77	3458	3.582	141.6
352	1961	2.844	101.2	3949	3.938	151.3
361	2236	2.823	100.8	4343	4.101	157.1
370	2598	2.632	97.24	4835	4.087	159.6
379	2996	2.254	90.8	5368	3.856	158.2
392	3636	1.836	88.48	6213	3.589	161.7
401	4014	1.875	96.45	6737	3.703	173
410	4471	2.145	112.5	7346	4.044	192.5
419	4780	2.601	132.4	7815	4.585	216.4
428	5013	3.126	153.7	8211	5.216	242.5
440	5222	3.944	184.7	8653	6.225	281.9
454	4700	4.365	193.9	8389	6.92	302.5
463	4224	4.403	189.8	8057	7.145	305.8
471	4163	4.659	197.4	8122	7.581	320.4
485	3993	5.016	206.5	8173	8.285	342.8
494	3872	5.036	206.2	8191	8.543	351.4
498	3798	5.122	207.4	8179	8.739	356.7
503	3728	5.127	207.1	8185	8.882	361.6
507	3628	5.044	203.1	8144	8.908	361.6

9/12/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
0	1126	0.1423	11.68	1126	0.1423	11.68
5	1095	0.1415	11.49	1116	0.1438	11.67
9	1100	0.1392	11.38	1137	0.1432	11.71
14	1252	0.155	12.8	1314	0.1614	13.32
18	1249	0.1506	12.61	1330	0.1589	13.29
23	1211	0.1425	11.99	1316	0.1529	12.85
29	1179	0.1351	11.61	1311	0.148	12.69
34	1153	0.1383	11.63	1307	0.1533	12.89
38	1157	0.1281	11.19	1329	0.1446	12.59
43	1181	0.136	11.65	1376	0.1546	13.23
47	1105	0.1335	11.16	1317	0.1537	12.88
52	1148	0.134	11.43	1382	0.1562	13.33

56	1116	0.1316	11.21	1366	0.1555	13.24
60	1094	0.13	10.99	1361	0.1555	13.16
69	1088	0.1308	11.02	1391	0.16	13.5
83	1058	0.1268	10.81	1417	0.1612	13.75
92	1032	0.1291	10.76	1426	0.1671	14
100	997.6	0.1317	10.73	1421	0.1728	14.23
109	978	0.1217	10.32	1434	0.1662	14.1
123	971.1	0.123	10.27	1476	0.1726	14.49
132	910.3	0.1182	9.837	1445	0.1711	14.32
144	909.3	0.1235	10.1	1482	0.1806	14.94
152	856.2	0.1191	9.711	1453	0.179	14.79
161	842.6	0.1146	9.511	1465	0.1777	14.84
170	851	0.122	9.939	1499	0.1882	15.52
179	808.5	0.1164	9.48	1481	0.1855	15.31
192	817.2	0.1218	9.825	1523	0.1953	16.01
201	762	0.1191	9.48	1490	0.1958	15.91
210	736.1	0.122	9.602	1486	0.2019	16.28
223	718	0.1209	9.524	1497	0.2056	16.56
232	716.2	0.1271	9.943	1514	0.215	17.23
241	697.9	0.1258	9.775	1514	0.2169	17.3
250	782.2	0.1493	11.44	1618	0.244	19.24
261	730.4	0.1556	11.47	1589	0.2549	19.6
274	678.6	0.1571	11.4	1562	0.2621	19.94
283	675.6	0.1686	11.98	1576	0.2778	20.8
292	680.7	0.1808	12.7	1596	0.2944	21.83
301	631.2	0.1761	12.18	1562	0.2941	21.59
310	633.3	0.1991	13.21	1579	0.3221	22.94
323	578	0.1962	12.81	1543	0.3264	23
332	558.3	0.2074	13.17	1537	0.3429	23.68
341	558.8	0.2144	13.61	1550	0.3553	24.44
350	550.9	0.2214	13.88	1554	0.3679	25.04
363	541.8	0.2387	14.52	1563	0.394	26.2
373	509.1	0.2409	14.32	1544	0.4031	26.38
382	519.6	0.2522	14.87	1567	0.4212	27.31
391	487.1	0.2536	14.66	1546	0.4289	27.45
400	469.1	0.2535	14.46	1539	0.4358	27.64
405	471.3	0.2598	14.79	1548	0.4458	28.17
409	473.3	0.2656	14.99	1555	0.4549	28.55
413	436.1	0.2633	14.52	1522	0.4558	28.24
418	439.2	0.248	14.04	1531	0.4441	27.96
422	434.9	0.2526	14.18	1531	0.4517	28.26

9/14/94						
Time(min)	**NA**	**VA**	**SA**	**NAcorr**	**VAcorr**	**SAcorr**
0	3994	0.9444	53.43	3994	0.9444	53.43
31	3790	0.4252	36.06	4246	0.4979	40.44
62	3551	0.3952	34.05	4481	0.508	41.98
90	3474	0.4326	35.93	4799	0.5778	46.71

121	3075	0.3854	32.07	4843	0.5671	46.08
152	4074	0.5812	46.72	6289	0.8136	64.81
179	4057	0.6168	49.15	6668	0.9023	71.31
212	3780	0.7283	54.52	6772	1.079	81.53
243	3832	1.002	69.36	7199	1.436	101.9
269	3875	1.422	89.83	7508	1.95	128.2
300	3453	2.181	115.7	7377	2.882	163.2
330	2639	2.574	122.5	6831	3.52	181.7
361	2277	3.236	137	6739	4.548	211.7
392	1948	3.875	147.4	6719	5.738	243.3
396	1866	3.888	145.6	6674	5.835	244.6
400	1763	3.779	140.3	6608	5.81	242.3
405	1726	3.835	140.2	6617	5.976	246.1
409	1643	3.796	137.5	6570	6.026	246.5
417	2146	4.07	145.1	7219	6.5	261.2

Table B.4. Time-dependent aerosol particle concentrations, volume concentrations, and surface area concentrations for *m*-xylene 1994 experiments.

NA, NB = particle number concentration not corrected for particle losses to walls (cm^{-3})
VA, VB = volume concentration not corrected for particle losses ($\mu m^3\ cm^{-3}$)
SA, SB = surface area concentration not corrected for particle losses ($\mu m^2\ cm^{-3}$)

NAcorr, NBcorr = particle number concentration corrected for particle losses (cm^{-3})
VAcorr, VBcorr = volume concentration corrected for particle losses ($\mu m^3\ cm^{-3}$)
SAcorr, SBcorr = surface area concentration corrected for particle losses ($\mu m^2\ cm^{-3}$)

8/19/94						
Time(min)	**NA**	**VA**	**SA**	**NAcorr**	**VAcorr**	**SAcorr**
0	728.7	0.1561	9.805	728.7	0.1561	9.805
5	694.9	0.1316	8.944	708.3	0.134	9.094
9	733.4	0.1289	9.09	758.1	0.1332	9.36
23	671.6	0.1417	8.945	732.3	0.1535	9.649
32	694.6	0.1405	9.152	780.1	0.1587	10.19
40	644.8	0.1243	8.621	749.7	0.1457	9.871
49	654.6	0.1382	9.444	779.4	0.1637	10.95
63	711	0.2211	14.11	864.2	0.2547	16.12
73	780.2	0.5247	27.28	954.6	0.5733	30.02
82	1044	1.086	45.59	1261	1.171	49.84
90	7939	2.206	105.6	8442	2.38	113.5
99	2.79E+04	6.439	426.6	2.93E+04	6.788	444.4
113	4.07E+04	25.9	1319	4.39E+04	27.14	1382
122	4.14E+04	41.04	1849	4.58E+04	43.71	1972
131	4.06E+04	55.11	2278	4.64E+04	60.06	2490
140	3.95E+04	66.24	2583	4.68E+04	74.3	2910
153	3.74E+04	76.76	2836	4.71E+04	90.47	3364
162	3.54E+04	78.96	2856	4.69E+04	97.06	3536
171	3.40E+04	79.39	2836	4.71E+04	102.1	3672
175	3.29E+04	78.67	2792	4.68E+04	103.4	3698
179	3.19E+04	77.45	2741	4.66E+04	104.2	3715
187	2.99E+04	75.05	2633	4.60E+04	105.8	3742
191	2.94E+04	74.26	2601	4.62E+04	107	3776
196	2.86E+04	72.45	2536	4.63E+04	107.6	3793
200	2.78E+04	71.18	2483	4.61E+04	108.2	3804
205	2.71E+04	69.97	2437	4.62E+04	109.3	3837
209	2.66E+04	69	2401	4.64E+04	110.2	3863
214	2.60E+04	67.57	2350	4.65E+04	111.1	3888
218	2.51E+04	65.68	2279	4.62E+04	111	3877
222	2.44E+04	64.24	2228	4.62E+04	111.3	3884
227	2.37E+04	62.84	2176	4.62E+04	112	3904

231	2.34E+04	62.2	2152	4.64E+04	113	3936
236	2.29E+04	60.78	2103	4.66E+04	113.7	3956
240	2.22E+04	59.21	2048	4.65E+04	113.7	3955
244	2.18E+04	58.31	2015	4.67E+04	114.4	3975
249	2.13E+04	57.13	1974	4.69E+04	115.2	3999
253	2.06E+04	55.25	1909	4.67E+04	114.8	3985
258	2.03E+04	54.51	1882	4.69E+04	115.9	4020
262	2.09E+04	56.31	1942	4.80E+04	119.3	4131
266	1.83E+04	49.22	1698	4.59E+04	113.5	3932
271	1.79E+04	48.14	1663	4.61E+04	114.1	3952
275	1.72E+04	46.45	1601	4.58E+04	113.7	3932
280	1.65E+04	44.45	1536	4.57E+04	113.2	3918
284	1.62E+04	43.56	1504	4.57E+04	113.5	3926
289	1.56E+04	42.2	1456	4.57E+04	113.6	3926
293	1.51E+04	40.69	1405	4.55E+04	113.2	3912
297	1.46E+04	39.64	1367	4.54E+04	113.2	3910
302	1.41E+04	38.34	1323	4.54E+04	113.2	3910
306	1.36E+04	36.87	1273	4.51E+04	112.7	3893
311	1.32E+04	35.75	1234	4.52E+04	112.8	3895
315	1.27E+04	34.6	1194	4.50E+04	112.6	3886
320	1.21E+04	33.11	1143	4.48E+04	112.3	3872
324	1.18E+04	32.1	1109	4.48E+04	112.1	3867
328	1.15E+04	31.35	1081	4.47E+04	112.2	3868
341	1.07E+04	28.65	995.4	4.49E+04	112	3866
346	1.69E+04	46.33	1598	5.16E+04	131.3	4522
350	1.49E+04	41.1	1416	5.00E+04	127.2	4377
355	1.43E+04	39.45	1360	4.98E+04	126.8	4365
359	1.38E+04	38.03	1311	4.97E+04	126.4	4351
364	1.32E+04	36.54	1259	4.95E+04	126.2	4340
368	1.27E+04	35	1208	4.93E+04	125.6	4321
372	1.24E+04	33.97	1173	4.93E+04	125.5	4316
377	1.21E+04	33.25	1148	4.94E+04	125.9	4329
381	1.16E+04	32.18	1109	4.92E+04	125.7	4319
386	1.13E+04	31.22	1076	4.92E+04	125.8	4321
390	1.10E+04	30.05	1039	4.92E+04	125.4	4311
395	1.06E+04	29.05	1003	4.91E+04	125.4	4308
399	1.02E+04	28.08	969.8	4.90E+04	125.2	4300
403	1.00E+04	27.7	955.5	4.91E+04	125.5	4311
408	9623	26.45	914.2	4.90E+04	125.2	4299
412	9266	25.38	878.1	4.88E+04	124.8	4286
417	9117	25.01	865.1	4.90E+04	125.2	4301
421	8831	24.2	836.9	4.89E+04	125.1	4294
426	8416	23.34	805	4.88E+04	125	4289
430	8085	22.32	770.7	4.86E+04	124.6	4274
435	7918	21.85	754.7	4.87E+04	124.8	4283
439	7646	21.04	727.7	4.86E+04	124.6	4275
443	7299	20.06	694.3	4.85E+04	124.1	4259
448	7102	19.65	678.5	4.85E+04	124.4	4265

452	6884	18.93	654.7	4.85E+04	124.2	4259
457	6720	18.39	637.4	4.85E+04	124.2	4262

8/21/94

Time(min)	NA	VA	SA	NAcorr	VAcorr	SAcorr
0	1753	0.266	20.47	1753	0.266	20.47
13	1888	0.2789	21.49	1979	0.29	22.33
21	1851	0.2849	21.68	2000	0.3242	23.69
30	1894	0.3407	23.49	2108	0.3967	26.4
39	1871	0.3467	23.64	2154	0.4393	28.02
53	1951	0.3146	23.35	2336	0.43	29.01
62	1848	0.4388	30.05	2284	0.5692	36.57
70	2029	0.7326	45.45	2509	0.8795	52.91
79	1996	1.446	74.39	2530	1.653	84.36
91	2001	3.662	142.5	2631	4.036	159
104	7563	4.455	169	8654	5.252	200.2
113	2.84E+04	6.32	409.9	3.05E+04	7.316	451.8
122	4.89E+04	24.22	1294	5.25E+04	25.84	1368
131	4.18E+04	38.66	1745	4.67E+04	41.59	1875
140	4.17E+04	58.63	2378	4.81E+04	64.06	2603
153	3.92E+04	76.79	2868	4.80E+04	87.66	3288
162	3.63E+04	80.6	2917	4.69E+04	95.95	3492
171	3.40E+04	81.41	2891	4.63E+04	101.5	3627
175	3.32E+04	81.17	2864	4.63E+04	103.4	3672
179	3.15E+04	79.31	2782	4.54E+04	103.6	3662
184	3.07E+04	78.16	2734	4.55E+04	105.1	3701
188	2.95E+04	75.85	2645	4.50E+04	104.8	3680
193	2.86E+04	74.69	2594	4.49E+04	106.1	3714
198	2.72E+04	72.37	2504	4.44E+04	106.3	3706
203	2.64E+04	70.77	2443	4.44E+04	107.1	3725
207	2.58E+04	69.84	2406	4.45E+04	108.1	3752
212	2.49E+04	67.18	2316	4.43E+04	107.7	3739
216	2.40E+04	65.04	2238	4.40E+04	107.3	3720
220	2.32E+04	63.29	2175	4.38E+04	107.3	3715
225	2.25E+04	61.9	2124	4.39E+04	108.1	3735
229	2.17E+04	59.58	2046	4.36E+04	107.4	3711
234	2.10E+04	57.93	1987	4.36E+04	107.7	3719
238	2.05E+04	56.38	1934	4.36E+04	107.8	3718
243	1.99E+04	55.06	1887	4.36E+04	108.3	3734
247	1.92E+04	52.92	1815	4.34E+04	107.7	3711
251	1.86E+04	51.28	1758	4.33E+04	107.4	3700
256	1.81E+04	49.88	1710	4.33E+04	107.8	3710
260	1.75E+04	48.28	1656	4.32E+04	107.5	3700
265	1.70E+04	46.46	1595	4.32E+04	107.3	3692
269	1.62E+04	44.74	1533	4.28E+04	106.8	3672
274	1.61E+04	44.64	1529	4.33E+04	108.2	3719
278	1.59E+04	44.09	1510	4.35E+04	108.9	3741

283	1.55E+04	42.58	1461	4.36E+04	108.9	3740
287	1.48E+04	40.95	1402	4.32E+04	108.4	3719
291	1.43E+04	39.56	1354	4.31E+04	108.1	3707
296	1.38E+04	37.95	1301	4.30E+04	107.8	3698
300	1.35E+04	37.27	1277	4.31E+04	108.1	3708
305	1.30E+04	35.94	1230	4.30E+04	108	3702
311	1.27E+04	34.6	1186	4.32E+04	108.1	3706
316	1.21E+04	33.35	1143	4.30E+04	108	3702
320	1.18E+04	32.39	1110	4.29E+04	108	3699
325	1.14E+04	31.14	1068	4.29E+04	107.8	3692
329	1.10E+04	30.35	1040	4.28E+04	107.9	3692
333	1.06E+04	29.04	996.3	4.27E+04	107.4	3675
338	1.02E+04	27.84	955.5	4.26E+04	107.1	3666
342	9773	26.57	913.2	4.24E+04	106.6	3648
347	9514	26.26	899.4	4.25E+04	107.2	3665
351	9192	25.13	861.8	4.24E+04	106.7	3650

9/4/94						
Time(min)	**NA**	**VA**	**SA**	**NAcorr**	**VAcorr**	**SAcorr**
0	2119	0.549	34.63	2119	0.549	34.63
9	2233	0.6438	39.79	2296	0.6612	40.8
22	1854	0.5122	31.78	2006	0.5553	34.24
31	1763	0.4416	28.62	1974	0.5148	32.41
40	1644	0.4341	27.49	1905	0.5213	32.08
49	1693	0.5566	32.77	2002	0.6612	38.3
63	1689	0.8062	45.44	2065	0.9466	52.78
71	1764	1.57	74.53	2186	1.751	83.69
80	2579	3.09	121.1	3109	3.386	134.8
95	4.77E+04	8.959	606.8	5.08E+04	9.727	646.1
104	7.38E+04	28.09	1649	7.92E+04	29.52	1726
112	8.07E+04	55.86	2790	8.80E+04	58.68	2935
121	8.08E+04	82.28	3701	9.06E+04	87.92	3966
130	7.89E+04	106.2	4423	9.13E+04	116.1	4855
139	7.63E+04	125.9	4958	9.17E+04	141.4	5601
153	7.09E+04	137	5168	9.11E+04	163.1	6193
161	6.84E+04	142.6	5270	9.13E+04	175.4	6530
170	6.59E+04	144.2	5258	9.19E+04	184.8	6792
184	6.77E+04	157.1	5634	9.90E+04	211.6	7646
188	6.33E+04	149	5324	9.61E+04	207.3	7467
192	5.96E+04	141.6	5044	9.37E+04	203.4	7311
197	5.80E+04	139.8	4962	9.38E+04	206.1	7382
201	5.66E+04	137.9	4882	9.36E+04	207.9	7423
207	5.41E+04	133.8	4717	9.31E+04	209	7436
211	5.25E+04	131	4607	9.27E+04	209.6	7443
216	5.18E+04	130	4564	9.36E+04	212.9	7544
220	5.01E+04	126.6	4435	9.30E+04	212.8	7528
225	4.83E+04	122.8	4297	9.26E+04	213.1	7528

229	4.66E+04	119.7	4177	9.21E+04	213.2	7516
233	4.50E+04	116.2	4050	9.16E+04	212.9	7493
238	4.34E+04	113.1	3931	9.12E+04	213.5	7501
242	4.21E+04	110.4	3830	9.10E+04	213.8	7500
247	4.01E+04	105.7	3663	9.02E+04	212.7	7453
251	3.86E+04	102.1	3534	8.97E+04	211.8	7417
256	3.71E+04	98.38	3403	8.93E+04	211.5	7397
260	3.60E+04	96.3	3324	8.92E+04	212	7406
264	3.48E+04	93.1	3212	8.87E+04	211.3	7379
269	3.33E+04	89.68	3088	8.83E+04	211	7358
273	3.22E+04	86.79	2989	8.80E+04	210.5	7338
278	3.14E+04	84.97	2922	8.82E+04	211.6	7368
282	3.01E+04	81.67	2807	8.77E+04	210.5	7328

10/20/94						
Time(min)	**NA**	**VA**	**SA**	**NAcorr**	**VAcorr**	**SAcorr**
0	7609	1.403	100.1	7609	1.403	100.1
9	7054	1.123	84.98	7298	1.156	87.4
25	7369	1.143	87.47	8052	1.231	94.07
33	7500	1.184	90.61	8404	1.301	99.39
42	7276	1.196	90.65	8419	1.345	101.8
51	7171	1.246	93.57	8536	1.428	107.2
60	6908	1.338	98.08	8479	1.556	114.3
69	6722	1.559	110	8472	1.816	128.9
82	6349	2.111	135.9	8328	2.441	159.4
91	6009	2.668	158.8	8130	3.065	186.1
100	5678	3.358	184.5	7938	3.844	216.5
113	5578	5.217	250.2	8053	5.909	291.8
122	5448	6.69	294.9	8092	7.607	346.1
131	5374	8.305	340.8	8209	9.537	404.7
141	5187	10.39	392.8	8265	12.14	475.6
150	4977	11.65	419.2	8298	13.99	523.2
163	4326	11.93	406.8	8013	15.33	546.5
168	4058	11.51	389.4	7878	15.33	542.6
172	3789	10.82	365.3	7709	14.95	528.7
176	3514	9.839	333.8	7525	14.25	506.5
181	3262	8.901	304.6	7376	13.63	487.7
185	3032	8.203	281.8	7223	13.16	472.5
190	2835	7.444	258.5	7112	12.65	457.6
194	2623	6.721	235.9	6963	12.11	440.9
199	2486	6.298	222.2	6899	11.89	434.3
203	2390	6.031	213.4	6860	11.78	430.7
207	2258	5.769	203.6	6781	11.66	425.9
212	2176	5.684	199.5	6765	11.76	428
216	2131	5.569	195.6	6771	11.79	429
221	2053	5.451	190.7	6756	11.84	430.1

225	1994	5.365	187.1	6745	11.9	431.2
229	1940	5.287	183.6	6740	11.95	432.3
234	1893	5.313	183	6753	12.16	437.7
238	1820	5.179	177.6	6727	12.16	436.9
243	1740	5.011	171.2	6704	12.16	436.2
249	1662	4.862	165.4	6693	12.21	437
253	1611	4.756	161.4	6684	12.23	437.3
258	1564	4.644	157.1	6690	12.28	438.3
262	1535	4.658	156.7	6703	12.43	442.2
266	1472	4.492	150.7	6680	12.39	440.4

11/9/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
0	2283	0.4292	30.65	2283	0.4292	30.65
4	1935	0.3583	25.73	1963	0.3628	26.04
9	1782	0.3281	23.54	1843	0.3379	24.21
13	1722	0.3081	22.21	1809	0.3218	23.16
22	1571	0.2798	20	1714	0.3019	21.53
31	1476	0.2524	18.41	1670	0.282	20.46
40	1383	0.2222	16.63	1625	0.2584	19.16
49	1373	0.2222	16.57	1661	0.2648	19.57
63	1268	0.217	16.09	1623	0.2693	19.79
72	1236	0.2195	16.03	1630	0.278	20.16
85	1238	0.2434	17.59	1684	0.3113	22.38
94	1240	0.2814	19.77	1721	0.3568	25.06
102	1227	0.372	24.42	1735	0.456	30.24
111	1247	0.4927	30.15	1785	0.5891	36.69
120	1271	0.7213	39.79	1839	0.8367	47.32
129	1207	0.9652	48.4	1806	1.108	57.24
143	1174	1.428	63.1	1828	1.639	74.91
151	1094	1.819	72.95	1784	2.094	87.27
160	1026	2.263	83.19	1763	2.647	101.4
174	866.7	2.444	83.21	1683	3.052	109
178	776	2.333	78	1613	3.008	106
182	708	2.142	71.29	1565	2.881	101.4
187	603.4	1.815	60.51	1481	2.621	92.77
191	528.9	1.562	52.32	1421	2.414	86.08
197	439.6	1.213	41.65	1349	2.116	77.09
202	377.1	0.9704	34.25	1298	1.905	70.76
206	338.6	0.8418	30.14	1267	1.797	67.36
211	321.9	0.7851	28.4	1259	1.763	66.43
215	295.9	0.7376	26.47	1240	1.733	65.11
220	290.6	0.7331	26.31	1243	1.749	65.7
224	281.4	0.7608	26.68	1241	1.796	66.72
228	270.7	0.7498	26.05	1237	1.803	66.73
233	268.5	0.7658	26.34	1244	1.844	67.86
237	253.2	0.7436	25.31	1235	1.841	67.49

242	257	0.7943	26.6	1248	1.919	69.69
246	255	0.7917	26.46	1253	1.939	70.27
251	246.3	0.7904	26.14	1253	1.965	70.87
255	226.5	0.7532	24.67	1240	1.95	70.12
259	220	0.7224	23.66	1240	1.94	69.79
264	215.5	0.695	22.81	1244	1.938	69.77
268	213.9	0.7194	23.38	1249	1.984	71.04
273	199	0.6646	21.61	1241	1.954	70.07
277	207.7	0.6903	22.39	1257	2.001	71.52
282	194.8	0.6606	21.39	1251	1.996	71.32
286	188.2	0.6364	20.6	1250	1.991	71.15
290	185.9	0.615	19.92	1254	1.989	71.08
295	178.7	0.5968	19.34	1253	1.993	71.23
299	178.3	0.589	19.06	1258	2.003	71.53
304	181	0.5921	19.14	1268	2.029	72.34
308	178.3	0.5836	18.99	1271	2.038	72.75
313	169.9	0.5669	18.35	1269	2.043	72.81
319	173.4	0.5616	18.26	1280	2.063	73.55
323	164.4	0.533	17.24	1276	2.051	73.04
328	158.3	0.5129	16.64	1276	2.05	73.08
332	160	0.5147	16.71	1283	2.068	73.64
336	156.6	0.5105	16.49	1284	2.079	73.93
341	149	0.4951	16.01	1282	2.083	74.06
345	153.4	0.4706	15.38	1291	2.072	73.88
350	160.8	0.4555	14.96	1304	2.074	74.02
354	170.7	0.4706	15.46	1319	2.104	74.98
359	164.1	0.4046	13.43	1318	2.053	73.44
363	178.9	0.4218	14.13	1337	2.082	74.55
367	171.4	0.3898	13.04	1335	2.062	73.83
372	188.4	0.4336	14.54	1358	2.122	75.86
376	195.6	0.4207	14.15	1370	2.121	75.87
381	179.3	0.4204	14.01	1360	2.137	76.25

Table B.5. Time-dependent aerosol particle concentrations, volume concentrations, and surface area concentrations for *p*-xylene 1994 experiments.

NA, NB = particle number concentration not corrected for particle losses to walls (cm^{-3})
VA, VB = volume concentration not corrected for particle losses ($\mu m^3\ cm^{-3}$)
SA, SB = surface area concentration not corrected for particle losses ($\mu m^2\ cm^{-3}$)

NAcorr, NBcorr = particle number concentration corrected for particle losses (cm^{-3})
VAcorr, VBcorr = volume concentration corrected for particle losses ($\mu m^3\ cm^{-3}$)
SAcorr, SBcorr = surface area concentration corrected for particle losses ($\mu m^2\ cm^{-3}$)

8/21/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
0	1353	0.1983	15.35	1353	0.1983	15.35
13	1276	0.184	14.37	1339	0.1919	14.97
21	1351	0.1869	15.02	1454	0.1993	15.98
30	1314	0.1875	14.84	1461	0.2051	16.22
39	1289	0.1787	14.33	1479	0.2013	16.11
53	1274	0.1728	13.92	1531	0.203	16.3
62	1239	0.1727	13.84	1537	0.2077	16.6
70	1219	0.1714	13.65	1552	0.2106	16.75
79	1188	0.1685	13.44	1560	0.2123	16.9
91	1133	0.1667	13.16	1554	0.2167	17.1
104	1109	0.1672	13.11	1582	0.2239	17.57
113	1117	0.1649	12.97	1625	0.2262	17.79
122	1080	0.1646	12.92	1622	0.2304	18.08
131	1215	0.1955	15.06	1793	0.2666	20.61
140	1170	0.1923	14.76	1784	0.2686	20.7
153	1129	0.1924	14.76	1791	0.2763	21.27
162	1169	0.2152	16.11	1863	0.3047	23.03
171	1146	0.2277	16.88	1872	0.3232	24.22
179	1130	0.2553	18.11	1881	0.357	25.87
193	1107	0.2892	19.82	1901	0.4021	28.31
203	741.5	0.228	15.08	1557	0.3474	24
212	851.6	0.3139	19.73	1686	0.4412	29.1
220	1141	0.5243	30.95	2000	0.6639	41
234	1145	0.7852	41.14	2050	0.9558	52.77
243	1751	1.017	49.49	2759	1.219	62.62
251	7708	1.322	67.37	9241	1.564	82.69
260	3.04E+04	2.212	156	3.38E+04	2.535	177.2
274	9.89E+04	8.111	718.8	1.08E+05	8.767	767.8
283	1.27E+05	14.87	1255	1.42E+05	15.94	1337
291	1.41E+05	23.32	1825	1.59E+05	24.95	1948
300	1.46E+05	34.1	2448	1.68E+05	36.55	2628

311	1.46E+05	48.96	3183	1.72E+05	52.81	3452
320	1.43E+05	62.84	3785	1.73E+05	68.18	4142
333	1.36E+05	82.3	4514	1.71E+05	90.55	5029
342	1.31E+05	98.55	5061	1.69E+05	109.5	5711
347	1.28E+05	104.2	5224	1.69E+05	116.8	5957
351	1.26E+05	109.6	5379	1.68E+05	123.7	6182

8/23/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
1	1088	0.1641	12.54	1092	0.1646	12.58
10	1398	0.2181	16.35	1451	0.225	16.86
23	1303	0.1948	14.84	1420	0.2099	15.95
32	1264	0.1871	14.35	1425	0.2078	15.87
41	1224	0.1808	13.86	1427	0.2067	15.78
50	1210	0.1757	13.6	1455	0.2068	15.9
63	1170	0.1674	13.11	1473	0.2054	15.95
72	1173	0.1677	13.09	1515	0.2106	16.3
83	1108	0.1632	12.63	1497	0.2119	16.27
92	1147	0.1654	12.97	1574	0.2187	16.98
100	1226	0.1735	13.71	1689	0.2312	18.05
109	1112	0.1568	12.48	1613	0.2191	17.18
123	1036	0.1445	11.59	1592	0.2136	16.81
132	997.8	0.1514	11.68	1587	0.2249	17.23
140	1016	0.159	12.07	1634	0.2363	17.9
149	961.7	0.1394	11.03	1611	0.2205	17.16
163	926.5	0.1437	11.11	1623	0.2312	17.72
172	866.1	0.1356	10.48	1590	0.2269	17.38
180	906.7	0.1401	10.91	1656	0.2349	18.07
189	861.7	0.1347	10.46	1638	0.2333	17.91
200	840	0.1366	10.55	1648	0.2396	18.34
209	795.5	0.1429	10.62	1628	0.2498	18.69
223	762.7	0.141	10.49	1629	0.2537	18.98
231	748.2	0.1401	10.58	1632	0.256	19.31
240	730.3	0.1559	11.24	1634	0.2759	20.26
249	716.2	0.1628	11.56	1638	0.287	20.86
263	867.9	0.2258	15.64	1818	0.3575	25.44
271	876.1	0.2657	17.76	1845	0.4035	27.94
280	858.9	0.3108	19.84	1848	0.4563	30.49
289	825.4	0.3716	22.29	1835	0.5266	33.49
302	1118	0.5018	27.1	2192	0.6749	39.27
312	3603	0.6542	35.65	4988	0.8481	49.07
321	1.00E+04	0.8509	54.08	1.22E+04	1.073	69.61
330	2.37E+04	1.245	101.7	2.76E+04	1.511	121.5
339	4.35E+04	2.323	222.4	4.99E+04	2.666	250
353	6.71E+04	5.99	554.7	7.76E+04	6.571	604.6
361	7.53E+04	9.767	831	8.80E+04	10.57	899.6
370	7.87E+04	14.08	1103	9.37E+04	15.23	1198

379	8.00E+04	19.45	1401	9.72E+04	21.07	1528
393	7.82E+04	27.96	1801	9.84E+04	30.56	1990
401	7.59E+04	33.48	2027	9.76E+04	36.8	2259
410	7.37E+04	39.75	2266	9.72E+04	44.06	2553
432	6.86E+04	56.17	2821	9.65E+04	63.94	3283
440	6.58E+04	61.41	2962	9.54E+04	70.82	3501
449	6.26E+04	65.71	3055	9.40E+04	77.2	3687
463	5.79E+04	70.32	3122	9.22E+04	85.48	3915
471	5.48E+04	71.91	3116	9.07E+04	89.37	4006
480	5.18E+04	72.94	3090	8.95E+04	93.15	4092
489	4.87E+04	73.14	3036	8.81E+04	96.21	4154
502	4.44E+04	73	2944	8.63E+04	100.5	4234
507	2.53E+04	38.41	1578	6.77E+04	66.75	2903
511	2.67E+04	41.01	1682	6.95E+04	70.11	3037
516	4.07E+04	71.7	2829	8.44E+04	102.6	4251
520	3.92E+04	70.59	2767	8.37E+04	102.9	4243
524	3.80E+04	69.84	2720	8.32E+04	103.5	4249
529	3.67E+04	68.8	2662	8.27E+04	104.2	4257
533	3.55E+04	67.44	2598	8.21E+04	104.3	4244

9/8/94						
Time(min)	**NA**	**VA**	**SA**	**NAcorr**	**VAcorr**	**SAcorr**
0	2113	0.2975	23.41	2113	0.2975	23.41
13	2343	0.2958	22.89	2471	0.3374	24.72
22	1893	0.2839	21.25	2086	0.3343	23.7
31	1817	0.2778	20.59	2077	0.3497	24.04
40	1756	0.2295	18.8	2074	0.3083	22.78
49	1653	0.2381	18.46	2029	0.3248	23
58	1790	0.7103	31.79	2231	0.8277	37.56
76	1558	0.1837	14.49	2101	0.3125	21.1
85	1263	0.1964	14.62	1847	0.3309	21.64
93	1195	0.1653	13.2	1819	0.304	20.57
102	1195	0.1767	13.49	1858	0.3206	21.23
111	1158	0.1647	13	1859	0.3132	21.1
120	1102	0.1496	12.17	1839	0.3026	20.62
133	1181	0.1634	13.04	1970	0.3223	21.97
142	1025	0.1622	12.48	1846	0.3256	21.75
151	1012	0.1622	12.62	1866	0.3307	22.26
160	984.3	0.1555	12.17	1867	0.3284	22.14
173	988.5	0.1755	13.21	1913	0.3564	23.72
190	987.6	0.1989	13.81	1973	0.3897	25.01
203	795.4	0.2079	14.39	1810	0.4065	26.09
212	836.9	0.2638	17.36	1879	0.4693	29.49
221	906.1	0.3107	19.66	1970	0.524	32.27
230	774.7	0.3654	21.39	1858	0.5884	34.53
243	1058	0.5896	30.43	2203	0.8418	44.91
252	1719	0.7043	35.25	2967	0.9792	50.86

261	2973	0.991	48.13	4395	1.301	65.46
270	4422	1.196	62.52	6067	1.552	82.11
283	6738	2.19	116.6	8748	2.661	141.6
292	8053	2.888	158.2	1.03E+04	3.474	188.5
302	1.44E+04	6.343	344.2	1.72E+04	7.19	386.5
311	1.53E+04	8.131	426	1.85E+04	9.268	481.6
320	1.53E+04	9.956	505.9	1.90E+04	11.42	576.7
333	1.54E+04	13.53	640	1.98E+04	15.61	738.4
342	1.53E+04	16.21	727.4	2.01E+04	18.86	850.2
346	1.49E+04	17.03	749	2.00E+04	19.98	883.8
351	1.49E+04	18.49	793	2.02E+04	21.84	944.4
355	1.47E+04	19.51	820.6	2.02E+04	23.22	986.3

9/12/94						
Time(min)	**NA**	**VA**	**SA**	**NAcorr**	**VAcorr**	**SAcorr**
0	1013	0.137	11.15	1013	0.137	11.15
9	1037	0.132	10.61	1072	0.1357	10.9
23	1332	0.1798	14.21	1437	0.1921	15.15
34	1856	0.5746	27.94	2052	0.6052	29.82
43	1379	0.1766	14.38	1623	0.2121	16.66
52	1341	0.1709	13.91	1633	0.2116	16.6
60	1737	0.1752	14.8	2087	0.22	17.85
69	1270	0.1674	13.64	1662	0.2169	17.07
83	1188	0.1581	12.87	1651	0.2215	17.15
92	1167	0.1499	12.33	1670	0.2173	16.94
100	934.3	0.1344	10.53	1465	0.2054	15.41
109	989	0.1332	10.8	1552	0.208	15.99
123	1273	0.1498	12.66	1891	0.2318	18.38
132	1002	0.1421	11.35	1652	0.2282	17.37
144	1008	0.1428	11.46	1700	0.234	17.89
152	913.3	0.1431	11.19	1631	0.238	17.91
161	918.3	0.1391	10.99	1663	0.2376	17.99
170	972.4	0.1507	11.97	1748	0.2547	19.36
179	920	0.1527	11.89	1721	0.2606	19.58
188	922.5	0.1594	12	1771	0.2732	20.1
201	885.8	0.1813	13.19	1778	0.3017	21.78
210	1144	0.3471	22.86	2062	0.4747	31.9
219	833.3	0.2033	14.19	1772	0.3363	23.59
228	1173	0.227	16.53	2140	0.3657	26.33
237	785.6	0.2555	16.48	1771	0.4009	26.69
246	785.6	0.2712	17.54	1795	0.4242	28.19
261	776.8	0.3677	21.68	1892	0.535	33.19
270	879.3	0.4637	26.08	2014	0.6432	38.24
279	770.7	0.5053	27.07	1926	0.699	39.96
292	744.1	0.6027	29.91	1933	0.8223	44.05
301	897.7	0.7206	34.22	2120	0.9622	49.37
310	973.9	0.85	37.84	2247	1.12	54.26

323	1307	0.9802	41.63	2685	1.305	60.39
332	1915	1.331	56.94	3392	1.707	77.8
341	2101	1.294	54.29	3687	1.729	77.53
350	2400	1.474	61.7	4096	1.98	87.75
363	2269	1.375	58.55	4109	1.994	88.87
373	2388	1.534	65.68	4332	2.24	99.35
382	2510	1.502	66.76	4545	2.29	103.5
391	2532	1.657	73.24	4656	2.536	113.4
400	2460	1.638	73.48	4664	2.607	117
405	2520	1.634	74.48	4774	2.651	119.9
409	2586	1.568	74.23	4874	2.62	121
413	2256	1.565	71.59	4575	2.654	119.7
418	2191	1.469	68.57	4546	2.601	118.3
422	2606	1.483	70.8	5001	2.648	121.9

9/21/94						
Time(min)	**NA**	**VA**	**SA**	**NAcorr**	**VAcorr**	**SAcorr**
0	2441	0.5465	35.82	2441	0.5465	35.82
5	2679	0.6805	43.34	2726	0.6922	44.03
9	2592	0.622	40.06	2675	0.6426	41.27
14	2796	0.5981	39.55	2941	0.6289	41.41
18	2356	0.5271	34.91	2535	0.5649	37.21
22	2333	0.4972	33.43	2545	0.5418	36.16
27	2362	0.5126	34.14	2616	0.5662	37.41
31	2368	0.4816	32.95	2656	0.5416	36.64
40	2503	0.4499	31.15	2889	0.5246	35.77
49	2170	0.4322	30.05	2629	0.52	35.53
63	2029	0.4074	28.36	2610	0.5157	35.18
72	1969	0.4168	28.2	2614	0.5374	35.81
84	1802	0.3889	26.35	2524	0.5253	34.97
93	1687	0.3522	24.08	2465	0.4995	33.41
102	2464	0.197	15.67	3410	0.3522	25.61
111	1351	0.2949	19.32	2379	0.4601	29.91
119	1568	0.3353	22.96	2647	0.51	34.15
133	1584	0.3416	23.29	2735	0.5313	35.45
142	1461	0.3133	21.5	2657	0.5124	34.26
151	1423	0.3081	21.12	2666	0.5167	34.5
160	1781	0.3078	21.12	3094	0.5255	35.11
173	1393	0.3274	21.81	2765	0.5585	36.64
182	1305	0.309	20.6	2716	0.5497	36.04
192	1325	0.3123	20.86	2782	0.5644	36.97
201	1372	0.333	22.18	2867	0.5947	38.88
210	1293	0.3271	21.67	2829	0.5991	39
219	1160	0.3147	20.24	2735	0.5961	38.14
232	1107	0.4803	24.24	2774	0.7886	43.29
241	1095	0.3675	22.62	2801	0.6868	42.29
250	1249	0.439	26.81	2987	0.771	47.19

263	1236	0.6012	32.22	3029	0.96	53.9
272	861.4	0.688	31.45	2681	1.071	54.18
281	1237	0.5874	33.08	3084	0.9881	56.69
289	780.6	0.562	27.76	2647	0.9787	52.1
303	1096	0.7491	38.82	3013	1.2	64.81
311	1061	0.8157	40.72	3005	1.295	67.92
320	1060	0.8955	43.54	3031	1.404	72.03
329	1006	0.9235	44	3007	1.464	73.93
345	899.5	0.9891	44.68	2950	1.591	77.27
354	1086	1.086	48.28	3167	1.729	82.56
363	821.7	1.084	46.43	2930	1.767	82.38
367	611.5	0.9105	37.34	2730	1.612	73.97
372	819.5	1.158	48.71	2953	1.886	86.38
376	838	1.196	49.95	2985	1.945	88.49
381	948.7	1.167	49.36	3114	1.944	88.97
385	779.4	1.192	48.8	2957	1.991	89.28
389	1110	1.169	48.11	3317	1.99	89.48

Table B.6. Time-dependent aerosol particle concentrations, volume concentrations, and surface area concentrations for *m*-ethyltoluene 1994 experiments.

NA, NB = particle number concentration not corrected for particle losses to walls (cm^{-3})
VA, VB = volume concentration not corrected for particle losses ($\mu m^3\ cm^{-3}$)
SA, SB = surface area concentration not corrected for particle losses ($\mu m^2\ cm^{-3}$)

NAcorr, NBcorr = particle number concentration corrected for particle losses (cm^{-3})
VAcorr, VBcorr = volume concentration corrected for particle losses ($\mu m^3\ cm^{-3}$)
SAcorr, SBcorr = surface area concentration corrected for particle losses ($\mu m^2\ cm^{-3}$)

9/6/94						
Time(min)	**NA**	**VA**	**SA**	**NAcorr**	**VAcorr**	**SAcorr**
0	1876	0.4796	26.79	1876	0.4796	26.79
4	1737	0.3961	23.58	1764	0.4044	23.98
8	1740	0.3455	22.16	1795	0.3604	22.9
13	1939	0.922	39.11	2037	0.9731	41.13
17	1743	0.575	28.47	1869	0.6419	31.1
22	1723	0.3351	21.59	1883	0.4101	24.65
26	1794	0.2984	20.34	1986	0.3786	23.7
30	1689	0.3488	21.55	1908	0.4364	25.27
35	1601	0.2886	19.64	1851	0.3824	23.72
39	1676	0.6975	31.09	1954	0.8128	35.95
44	1679	0.2912	19.7	1997	0.4127	24.92
48	1574	0.3048	20.08	1916	0.4319	25.6

53	1614	0.7142	32.64	1988	0.8642	39.05
57	1536	0.2582	19.33	1932	0.4115	25.97
62	1511	0.3009	20.87	1931	0.4599	27.85
66	1569	0.4	24.78	2010	0.5662	32.13
71	1576	0.4446	27.39	2041	0.6206	35.22
75	1580	0.4339	28.65	2062	0.6158	36.83
79	1562	0.4873	31.57	2061	0.6754	40.11
86	1610	0.6833	40.56	2139	0.8868	49.94
91	1540	0.875	48.2	2090	1.093	58.31
95	1560	1.201	60.5	2129	1.437	71.42
100	1545	1.593	73.88	2138	1.859	86.13
104	1585	2.206	92.22	2205	2.512	106.1
108	1778	2.927	111.4	2440	3.297	127.6
113	2763	3.603	130.4	3529	4.088	150.6
117	5353	3.927	146.9	6275	4.522	171
122	1.01E+04	3.581	170.2	1.13E+04	4.286	198.7
126	1.64E+04	4.363	257	1.80E+04	5.143	289.4
131	2.30E+04	7.535	439.6	2.50E+04	8.451	479.3
135	2.78E+04	12.35	669.9	3.02E+04	13.45	718.7
140	3.03E+04	17.66	894.6	3.33E+04	19.1	959.3
144	3.21E+04	24.03	1138	3.55E+04	25.88	1220
149	3.25E+04	30.13	1352	3.65E+04	32.66	1463
153	3.22E+04	36.16	1546	3.67E+04	39.39	1684
158	3.19E+04	41.08	1695	3.69E+04	45.38	1873
162	3.12E+04	45.29	1816	3.68E+04	50.57	2030
166	3.04E+04	49	1916	3.65E+04	55.37	2170
171	3.11E+04	53.62	2064	3.79E+04	61.52	2373
175	4.39E+04	83.68	3136	5.16E+04	93.58	3516
180	4.19E+04	85.06	3143	5.06E+04	97.54	3613
184	4.03E+04	86.12	3143	4.99E+04	100.7	3688
189	3.85E+04	85.98	3105	4.91E+04	103.3	3742
193	3.72E+04	86.26	3088	4.87E+04	105.8	3802
200	3.50E+04	84.49	2996	4.79E+04	107.9	3840
204	3.37E+04	82.8	2921	4.74E+04	108.4	3839
209	3.24E+04	80.76	2841	4.69E+04	109	3848
213	3.07E+04	77.9	2729	4.60E+04	108.2	3806
218	2.91E+04	74.58	2606	4.53E+04	107.3	3767
222	2.43E+04	62.66	2185	4.10E+04	97.08	3402
226	2.29E+04	59.29	2068	4.02E+04	95.28	3338
231	2.20E+04	57.41	1998	4.00E+04	95.33	3333
235	2.06E+04	54.4	1891	3.92E+04	93.77	3274
240	1.96E+04	51.95	1804	3.87E+04	93.07	3246
244	1.88E+04	49.92	1733	3.84E+04	92.37	3220
249	1.78E+04	47.5	1646	3.79E+04	91.54	3187
253	1.71E+04	45.52	1579	3.76E+04	90.78	3160
257	1.63E+04	43.86	1519	3.73E+04	90.29	3140
262	1.56E+04	41.97	1454	3.70E+04	89.81	3122
266	1.51E+04	40.71	1408	3.69E+04	89.64	3113

271	1.43E+04	38.54	1335	3.65E+04	88.76	3083
275	1.38E+04	37.61	1299	3.64E+04	88.84	3081
279	1.34E+04	37.07	1276	3.63E+04	89.31	3091
284	1.26E+04	34.15	1183	3.59E+04	87.52	3036
288	1.20E+04	32.71	1132	3.57E+04	86.95	3015
293	1.16E+04	31.41	1088	3.56E+04	86.69	3006
297	1.11E+04	30.47	1053	3.54E+04	86.57	2998
302	1.06E+04	29	1001	3.52E+04	86.07	2979
306	9980	27.46	948	3.48E+04	85.26	2951
312	9418	26.07	899.1	3.46E+04	84.91	2937
317	8928	24.79	854.8	3.44E+04	84.46	2920
321	8683	24.09	830.6	3.44E+04	84.41	2918
326	8448	23.52	810.5	3.44E+04	84.62	2924
330	8066	22.62	777.9	3.43E+04	84.32	2912
335	7690	21.65	743.7	3.41E+04	84.09	2902
339	7399	20.84	715.8	3.40E+04	83.83	2893
344	7086	20.03	687.4	3.39E+04	83.69	2887
348	7092	20.02	687.8	3.41E+04	84.21	2905
352	6965	19.77	678.3	3.42E+04	84.5	2914
357	6675	18.77	643.1	3.41E+04	84.13	2900
361	6346	18.09	619.9	3.40E+04	83.93	2893
366	6015	17.19	588.9	3.38E+04	83.62	2881
370	5814	16.45	563.3	3.38E+04	83.31	2870
375	5560	15.89	544.3	3.37E+04	83.29	2869
379	5360	15.46	528.3	3.36E+04	83.28	2867
384	5030	14.51	495.8	3.35E+04	82.81	2851
388	4867	14.09	481.3	3.34E+04	82.77	2849
392	4710	13.61	465.1	3.34E+04	82.66	2845
397	4458	12.95	441.4	3.33E+04	82.43	2836
401	4252	12.32	419.1	3.32E+04	82.14	2825
406	4113	11.93	406.9	3.32E+04	82.15	2826
410	3893	11.46	389.1	3.31E+04	81.99	2819
415	3687	10.8	367.1	3.30E+04	81.7	2809
419	3606	10.67	361.7	3.30E+04	81.86	2814
424	3448	10.23	346.8	3.30E+04	81.78	2810
428	3310	9.811	332.5	3.29E+04	81.62	2805
436	3070	9.069	307.3	3.29E+04	81.38	2796
440	2908	8.597	291.1	3.28E+04	81.14	2788
445	2847	8.391	284.2	3.28E+04	81.22	2791
449	2753	8.236	278.2	3.28E+04	81.3	2792
454	2572	7.721	260.7	3.27E+04	81.05	2783
458	2503	7.504	253	3.27E+04	81.04	2783
463	2410	7.317	246.2	3.27E+04	81.1	2784
467	2231	6.682	225.4	3.26E+04	80.65	2770
471	2174	6.496	219	3.26E+04	80.65	2769
476	2180	6.194	209	3.27E+04	80.56	2766
480	1983	5.881	198.7	3.25E+04	80.41	2761
485	1900	5.709	192.2	3.25E+04	80.43	2761

489	1823	5.481	184.7	3.25E+04	80.36	2759
494	1763	5.237	176.2	3.25E+04	80.3	2757
498	1664	4.988	167.9	3.24E+04	80.19	2753
503	1636	4.941	166	3.24E+04	80.31	2757
507	1729	4.821	162.7	3.26E+04	80.32	2758

9/10/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
1	1699	0.2405	19.11	1705	0.2413	19.17
5	1579	0.222	17.71	1609	0.2254	17.98
10	1598	0.2447	18.65	1657	0.252	19.22
14	1569	0.2298	17.89	1651	0.24	18.67
19	1549	0.2315	17.93	1660	0.2454	18.99
23	1515	0.2244	17.57	1648	0.2411	18.84
28	1514	0.2258	17.55	1674	0.246	19.09
32	1549	0.2226	17.7	1731	0.2455	19.46
36	1490	0.2199	17.37	1693	0.2454	19.34
41	1510	0.2262	17.72	1740	0.2551	19.95
45	1508	0.2355	18.25	1759	0.2673	20.7
50	1493	0.2461	18.76	1770	0.2817	21.49
54	1497	0.249	19.03	1793	0.2877	21.98
59	1466	0.2592	19.65	1786	0.3017	22.89
63	1548	0.3	22.07	1887	0.3462	25.56
68	1516	0.3188	23.24	1877	0.3697	27.06
72	1491	0.371	25.79	1868	0.4262	29.89
76	1560	0.4524	30.4	1953	0.5129	34.84
81	1559	0.5726	35.94	1973	0.6415	40.88
85	1583	0.7066	42.14	2014	0.7841	47.56
93	1590	1.146	59.42	2056	1.255	66.33
98	1928	1.977	92.23	2425	2.123	100.8
102	1911	2.505	108.7	2437	2.693	119
106	1878	3.309	130.7	2438	3.562	143.5
111	1897	4.2	153.6	2510	4.574	170.7
115	1910	4.75	163.3	2575	5.251	184.6
120	2186	4.953	164.8	2933	5.641	192.2
124	2739	3.813	131.6	3565	4.617	162.9
129	4355	2.445	104.3	5307	3.323	138.3
133	7147	2.678	137.1	8241	3.603	173.4
138	1.05E+04	4.109	215.2	1.18E+04	5.122	255.6
142	1.39E+04	6.327	324.7	1.55E+04	7.448	370.2
147	1.74E+04	9.967	487.6	1.93E+04	11.31	542.7
151	2.03E+04	14.98	692.2	2.25E+04	16.6	758.8
155	2.18E+04	19.39	860.9	2.44E+04	21.38	942.6
160	2.30E+04	25.54	1078	2.60E+04	28.19	1184
164	2.33E+04	30.86	1250	2.66E+04	34.18	1381
169	2.30E+04	34.91	1372	2.68E+04	39.22	1539
173	2.24E+04	38.67	1477	2.67E+04	43.88	1677

178	2.18E+04	41.14	1540	2.66E+04	47.58	1783
182	2.08E+04	42.43	1561	2.61E+04	49.92	1841
187	1.99E+04	43.45	1573	2.57E+04	52.3	1900
191	1.89E+04	43.66	1561	2.51E+04	53.64	1926
195	1.80E+04	43.32	1535	2.46E+04	54.42	1938
200	1.71E+04	42.66	1499	2.42E+04	55.18	1950
206	1.58E+04	40.8	1423	2.35E+04	54.95	1929
211	1.50E+04	39.38	1367	2.31E+04	54.85	1918
215	1.43E+04	38.08	1318	2.27E+04	54.59	1903
220	1.36E+04	36.74	1269	2.25E+04	54.49	1896
224	1.29E+04	35.3	1217	2.22E+04	54.01	1876
228	1.22E+04	33.32	1149	2.17E+04	52.93	1837
233	1.16E+04	31.95	1099	2.15E+04	52.64	1824
237	1.10E+04	30.55	1051	2.12E+04	52.07	1804
242	1.04E+04	29.02	998.6	2.09E+04	51.52	1784
246	9963	27.92	959.8	2.07E+04	51.18	1771
251	9556	26.92	924.2	2.06E+04	51.09	1765
255	9087	25.6	879.7	2.04E+04	50.45	1744
260	8673	24.54	842.8	2.03E+04	50.22	1735
264	8288	23.59	809.3	2.01E+04	49.9	1723
268	7901	22.56	774	1.99E+04	49.48	1708
273	7605	21.81	747.6	1.99E+04	49.46	1706
277	7291	21.01	719.1	1.97E+04	49.22	1696
282	7060	20.42	698.6	1.97E+04	49.31	1698
286	6763	19.59	670.2	1.96E+04	49.01	1688
291	6854	20.07	684.6	1.99E+04	50.17	1725
295	6779	19.89	678.3	2.00E+04	50.52	1736
299	6524	19.33	657.5	2.00E+04	50.48	1733
304	6193	18.32	623.6	1.98E+04	50.09	1720
308	5979	17.85	606.2	1.98E+04	50.1	1719
313	5747	17.24	584.8	1.97E+04	50.08	1717
318	5408	16.42	555.1	1.96E+04	49.82	1706
323	5138	15.58	527	1.95E+04	49.51	1695
327	5042	15.37	519.1	1.95E+04	49.72	1701
332	4784	14.61	493.2	1.94E+04	49.46	1692
336	4635	14.27	480.9	1.94E+04	49.51	1693
341	4456	13.8	464	1.94E+04	49.51	1692
345	4313	13.36	449.4	1.94E+04	49.44	1689
349	4132	12.89	432.9	1.93E+04	49.33	1685
354	3920	12.26	411.4	1.92E+04	49.13	1677

9/19/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
1	1004	0.1245	10.2	1008	0.1249	10.24
5	1032	0.1325	10.59	1051	0.1347	10.76
10	986.2	0.121	9.987	1025	0.1251	10.31
14	970.2	0.1207	9.819	1024	0.1265	10.27

19	952.7	0.118	9.597	1025	0.1257	10.21
23	959.3	0.1136	9.499	1046	0.1227	10.23
28	938	0.1122	9.387	1043	0.1231	10.26
32	916.3	0.1109	9.221	1035	0.1232	10.21
37	904.2	0.1062	8.981	1040	0.1201	10.12
41	892.3	0.1065	9.023	1042	0.1218	10.27
46	887.7	0.1117	9.289	1053	0.1288	10.68
50	238.7	4.13E-02	3.006	407.6	5.89E-02	4.434
58	864.7	0.1217	9.906	1056	0.1421	11.57
63	871.2	0.1256	10.3	1077	0.1478	12.11
67	888.5	0.1356	10.97	1105	0.1595	12.9
72	890	0.1595	12.22	1120	0.1857	14.33
76	920.7	0.1905	13.99	1161	0.219	16.26
80	878.6	0.2066	14.77	1129	0.2376	17.2
85	915.4	0.2571	17.46	1178	0.2918	20.13
89	918.4	0.2861	19.01	1190	0.3241	21.89
94	927.3	0.3562	22.28	1211	0.3995	25.47
98	952.4	0.4399	26.21	1246	0.4884	29.69
103	1080	0.6164	34.51	1387	0.6744	38.48
107	1080	0.7476	39.47	1399	0.8154	43.93
112	1081	0.9141	45.46	1417	0.9976	50.66
116	1046	1.077	50.43	1395	1.177	56.34
120	1090	1.382	60.71	1455	1.504	67.56
125	1054	1.628	67.31	1440	1.787	75.62
129	1022	1.92	74.61	1428	2.117	84.37
134	993.9	2.212	81.5	1425	2.472	93.5
138	988.8	2.52	88.99	1444	2.842	103.1
143	947.1	2.718	92.36	1433	3.133	109.6
147	876	2.734	90.15	1387	3.229	110
151	776.1	2.457	80.38	1310	3.028	102.7
156	601.8	1.75	58.24	1157	2.388	82.7
160	509.2	1.274	44.28	1077	1.947	69.9
165	449.8	0.9243	34.15	1030	1.624	60.72
173	492.7	0.9254	34.57	1094	1.665	62.61
177	586.8	1.13	41.23	1201	1.896	70.2
182	677.1	1.328	47.48	1311	2.134	77.89
186	750.6	1.482	52.22	1402	2.327	83.94
191	800.7	1.527	53.65	1475	2.424	87.13
195	868.2	1.668	58.06	1563	2.613	93.1
200	932.4	1.799	62.55	1654	2.808	99.74
204	973	1.767	62.29	1717	2.826	101.2
208	981.2	1.771	62.93	1746	2.88	103.5
213	1005	1.77	63.81	1796	2.94	106.4
217	1005	1.744	63.63	1817	2.961	107.8
222	1009	1.765	65.01	1845	3.04	111.2
226	993.7	1.741	64.5	1850	3.06	112.2
231	1009	1.807	66.74	1890	3.183	116.4
235	1023	1.884	69.53	1926	3.307	120.8

240	982.8	1.844	67.96	1910	3.324	121.2
244	969.6	1.925	70.11	1917	3.454	125.1
249	949.4	1.933	70.15	1921	3.522	127.2
253	914.7	1.899	68.74	1906	3.536	127.5
257	904.3	1.932	69.37	1915	3.619	129.8
262	921.8	2.074	73.6	1958	3.828	136.3
266	875.6	2.002	70.95	1932	3.809	135.5
271	855.8	1.992	70.37	1936	3.864	137.1
275	852.5	2.008	70.63	1952	3.934	139.2
280	828.7	1.996	69.94	1953	3.988	140.7
288	792.3	1.975	68.7	1954	4.074	143.1
292	797.8	1.856	65.03	1978	4.005	141.1
297	753.2	1.838	64.22	1956	4.048	142.4
301	766	1.932	67.16	1987	4.195	147
306	722.2	1.821	63.37	1965	4.146	145.3
310	748.3	1.905	66.11	2009	4.281	149.8
315	736.9	1.859	64.62	2020	4.297	150.4
319	734.7	1.831	63.84	2035	4.318	151.3

10/6/94						
Time(min)	**NA**	**VA**	**SA**	**NAcorr**	**VAcorr**	**SAcorr**
0	3866	2.16	89.28	3866	2.16	89.28
4	2.76E+04	16.32	767.3	2.80E+04	16.64	780.6
9	3256	0.5455	39.42	3749	0.8757	53.36
13	3238	0.5191	37.92	3783	0.8565	52.35
18	3180	0.4883	36.27	3788	0.834	51.29
22	3169	0.4838	35.92	3829	0.8361	51.41
27	3411	0.5203	39.79	4138	0.8807	55.89
31	2961	0.4265	32.6	3736	0.7926	49.12
36	2900	0.4195	31.93	3734	0.7925	48.97
40	2907	0.4076	31.36	3788	0.7861	48.8
45	3147	0.6877	40.11	4106	1.083	58.39
49	2852	0.3803	29.96	3859	0.7802	48.62
54	2804	0.409	30.99	3867	0.8159	50.15
58	2964	0.3929	31.18	4074	0.8049	50.75
62	2774	0.3864	30.13	3929	0.8033	50.07
67	2832	0.4041	31.5	4042	0.8275	51.94
71	3290	0.4829	37.69	4549	0.9121	58.59
76	3941	0.5481	42.77	5291	0.9858	64.34
83	3773	0.7344	50.87	5213	1.192	73.62
88	4307	0.8749	59.31	5821	1.35	83.07
92	4051	0.9075	61.7	5616	1.396	86.25
97	4267	0.993	69.65	5893	1.496	95.18
101	4287	1.213	80.27	5961	1.732	106.7
106	5097	1.691	100.6	6908	2.241	128.7
110	4298	1.563	97.38	6154	2.132	126.6
115	4248	1.924	113	6160	2.523	143.9

119	4955	2.235	126.4	6968	2.864	158.8
123	3890	2.372	128.3	5945	3.032	162.3
128	3795	2.687	139	5904	3.393	175.2
132	4241	3.172	157.2	6411	3.925	195.6
137	3772	3.55	168	6004	4.369	209.4
141	3093	3.518	158.7	5368	4.394	202.4
146	2505	3.433	146.4	4827	4.384	193.2
150	3264	4.116	167.4	5678	5.146	217.3
154	2409	4.424	172.6	4867	5.544	225.8
159	2250	4.836	179.6	4766	6.091	237.7
163	2216	5.179	185.7	4785	6.561	248.2
168	1891	5.375	183.2	4521	6.939	251.9
172	1730	5.406	178.7	4408	7.129	252.5
176	1421	4.612	150.4	4142	6.478	228.7
181	1873	4.07	136.2	4699	6.089	219.5
185	1109	3.404	112.7	3965	5.527	199.4
190	847.4	2.295	79	3731	4.498	168.3
197	662.8	1.522	56.01	3572	3.785	147.5
201	857.7	2.589	87.21	3790	4.925	181.1
205	608.6	1.533	55.18	3555	3.904	150.3
210	805.7	1.865	64	3778	4.295	161.1
214	562.2	1.756	58.83	3551	4.233	157.6
219	531.5	1.764	57.74	3541	4.304	158.5
223	525.5	1.81	58.2	3551	4.405	160.8
228	505.4	1.786	56.49	3552	4.452	161.3
232	468.8	1.619	50.81	3531	4.338	157.3
237	877.7	1.336	43.41	3971	4.11	151.6
241	544	1.024	33.55	3653	3.829	142.8
246	402.4	0.8553	28.88	3525	3.692	139.2
250	421.2	0.6901	24.73	3553	3.545	135.6
254	837.8	0.695	26.24	3991	3.568	137.8
259	540	0.8244	29.92	3708	3.724	142.4
263	582.7	0.7739	29.12	3763	3.692	142.3
268	850.7	0.83	31.82	4055	3.775	145.9
272	816.4	0.9893	37.66	4037	3.959	152.6
277	889.6	1.081	41.4	4133	4.085	157.6
281	1087	1.294	49.78	4352	4.331	167.1
286	1412	1.417	55.72	4708	4.498	174.7
290	1185	1.574	60.47	4504	4.695	180.8
294	1223	1.692	65.26	4564	4.855	187.1
299	1634	1.884	73.8	5034	5.103	197.6
308	1279	2.022	77.04	4734	5.352	204.8
312	1317	2.09	79.9	4798	5.47	209.4
317	1156	2.023	76.06	4665	5.464	207.7
321	1114	2.048	76.17	4645	5.539	209.6
326	1137	2.167	79.96	4698	5.725	215.7
330	1151	2.194	80.49	4736	5.807	218.1
335	1071	2.226	80.64	4685	5.909	220.7

339	1029	2.21	79.42	4666	5.949	221.4
343	1159	2.167	77.68	4830	5.961	221.6

10/20/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
0	1474	0.2026	16.49	1474	0.2026	16.49
5	1418	0.1963	15.83	1444	0.1993	16.06
9	1376	0.1891	15.42	1421	0.1943	15.85
14	1378	0.1901	15.41	1448	0.1982	16.07
18	1391	0.1949	15.75	1481	0.2054	16.6
25	1369	0.1794	14.91	1494	0.1935	16.06
29	1324	0.1861	15.04	1468	0.2024	16.38
33	1300	0.1812	14.78	1462	0.1997	16.29
38	1316	0.1845	14.99	1501	0.2057	16.72
42	1282	0.1774	14.53	1484	0.2007	16.44
47	1317	0.184	14.96	1543	0.2099	17.09
51	1288	0.1831	14.84	1532	0.2112	17.14
56	1265	0.185	14.96	1530	0.2158	17.48
60	1287	0.1992	15.67	1570	0.2324	18.37
65	1240	0.1836	14.83	1543	0.2194	17.74
69	1247	0.1955	15.55	1567	0.2335	18.64
74	1261	0.2109	16.45	1600	0.252	19.77
78	1266	0.2282	17.31	1621	0.272	20.83
82	1312	0.2402	18.35	1682	0.2868	22.08
87	1254	0.24	18.21	1643	0.29	22.19
91	1335	0.2892	21.15	1739	0.3424	25.36
96	1316	0.308	22.06	1738	0.3655	26.57
100	1275	0.3237	22.72	1711	0.3849	27.48
105	1309	0.3657	25.05	1762	0.432	30.14
109	1315	0.4033	26.97	1782	0.4742	32.35
113	1296	0.437	28.42	1776	0.5129	34.11
118	1307	0.5118	31.89	1804	0.5949	38.01
122	1322	0.5802	34.95	1832	0.6701	41.46
127	1331	0.6598	38.37	1859	0.7596	45.42
131	1355	0.7571	42.53	1897	0.8662	50.08
137	1340	0.8719	46.82	1904	0.9978	55.21
141	1313	0.9785	50.44	1892	1.117	59.47
146	1316	1.089	54.49	1915	1.246	64.4
150	1309	1.185	57.65	1924	1.359	68.33
154	1319	1.325	62.45	1951	1.519	74
159	1286	1.48	67.04	1940	1.703	79.83
163	1628	2.051	90.14	2305	2.307	104.3
168	1700	2.378	101.3	2410	2.685	117.5
172	1674	2.567	106.1	2410	2.92	124.2
176	1648	2.786	111.8	2413	3.193	132
181	1645	3.029	118.3	2448	3.511	141.3
185	1611	3.282	124.3	2446	3.834	149.9

190	1598	3.577	131.6	2475	4.23	160.8
194	1570	3.807	136.5	2482	4.552	168.9
199	1508	3.898	136.8	2465	4.766	173.5
203	1492	4.142	142.3	2487	5.121	182.6
207	1448	4.246	143.3	2482	5.343	187.5
212	1370	4.21	139.9	2451	5.459	189.2
216	1299	4.123	135.5	2418	5.496	188.8
221	1190	3.852	125.7	2353	5.373	183.7
225	1052	3.367	110.1	2246	4.993	171.4
229	977.1	3.035	99.98	2199	4.754	164.3
234	828.8	2.399	80.69	2078	4.207	147.9
238	714.8	1.942	66.86	1982	3.805	135.9
243	665.1	1.624	58.08	1952	3.539	128.9
249	593.7	1.353	49.81	1899	3.314	122.3
253	566.7	1.259	46.92	1884	3.248	120.4
258	574.5	1.318	48.78	1908	3.342	123.5
262	558.2	1.305	47.94	1903	3.357	123.7
266	549.2	1.371	49.45	1907	3.454	126.3

11/4/94						
Time(min)	**NA**	**VA**	**SA**	**NAcorr**	**VAcorr**	**SAcorr**
0	3232	0.5158	38.44	3232	0.5158	38.44
5	2960	0.4425	33.79	3019	0.4494	34.32
9	2963	0.4308	33.24	3069	0.4431	34.18
14	2957	0.4102	32.27	3122	0.4289	33.72
18	2907	0.4078	31.99	3117	0.4316	33.83
23	2879	0.4106	32.15	3146	0.4407	34.48
27	2833	0.3996	31.56	3144	0.4344	34.28
32	2805	0.4047	31.44	3171	0.446	34.65
36	2763	0.3873	30.64	3171	0.4333	34.22
40	2741	0.4004	30.9	3193	0.4514	34.87
45	2707	0.3929	30.57	3211	0.4501	35.01
49	2640	0.3879	29.96	3185	0.45	34.77
54	2662	0.3824	30	3258	0.4503	35.27
58	2618	0.3774	29.67	3254	0.4499	35.3
63	2651	0.3978	30.77	3337	0.4765	36.87
67	2633	0.3988	30.87	3357	0.4823	37.35
72	2674	0.4152	31.98	3447	0.505	38.93
76	2627	0.4163	31.7	3438	0.5112	39.04
85	2556	0.4136	31.73	3448	0.5197	39.91
90	2550	0.4395	33.08	3485	0.5523	41.76
94	2563	0.4556	34.31	3532	0.5737	43.38
99	2588	0.5164	37.54	3597	0.6423	47.15
103	2569	0.5481	39.32	3609	0.6804	49.37
108	2558	0.6212	43.05	3634	0.7627	53.72
112	2622	0.7319	48.88	3728	0.8822	60.1
117	2565	0.8023	52.36	3705	0.9644	64.31

121	2590	0.989	61.13	3756	1.163	73.76
125	2610	1.247	72.17	3804	1.437	85.65
130	2620	1.581	85.3	3850	1.797	100.1
134	2537	1.911	96.98	3797	2.154	113
139	2520	2.383	113.2	3820	2.671	131.2
143	2441	2.892	128.3	3774	3.228	148.4
148	2391	3.378	142.2	3771	3.789	165.3
152	2341	3.922	156.6	3761	4.411	182.7
157	2256	4.62	173.5	3733	5.238	204.2
161	2162	5.065	182.7	3686	5.805	217.6
165	2066	5.319	186.3	3640	6.196	225.9
170	1852	5.304	179.8	3486	6.365	225.5
174	1617	4.901	163.2	3296	6.106	213.7
179	1419	4.321	143.6	3147	5.686	199.2
183	1229	3.633	121.8	2991	5.105	180.9
188	1034	2.846	97.71	2828	4.416	160.1
192	897	2.367	82.86	2713	3.999	147.3
199	783.1	2.045	72.24	2632	3.765	139.7
203	770.7	2.163	74.88	2639	3.938	144.3
207	729.8	2.131	72.88	2618	3.962	144.2
212	703.7	2.14	72.29	2616	4.043	146
216	693.2	2.213	73.34	2625	4.179	149.1
221	636	2.166	70.66	2592	4.211	149
225	610.2	2.12	68.67	2586	4.229	149.1
230	558.2	1.991	63.93	2556	4.176	146.8
234	518.4	1.809	58.34	2532	4.049	142.9
238	458	1.597	51.64	2486	3.886	137.8
243	426.9	1.436	46.81	2471	3.778	134.7
247	381.2	1.266	41.49	2437	3.646	130.6
252	355.5	1.17	38.45	2425	3.591	128.9
256	340.1	1.111	36.56	2419	3.563	128.1
261	314.6	1.029	33.84	2405	3.518	126.5
265	300.1	1.019	33.25	2400	3.538	126.9
269	299.6	1.029	33.46	2408	3.578	128.1
274	288.1	0.9881	32.03	2408	3.573	127.8
278	274.8	0.9727	31.14	2403	3.588	127.9
283	272.2	0.957	30.61	2412	3.609	128.6
287	241.8	0.8504	27.28	2389	3.528	126.1
292	244.2	0.8946	28.35	2402	3.607	128.3
296	225.5	0.8194	26.03	2390	3.558	126.7
300	211.8	0.7866	24.79	2383	3.55	126.3
305	193.6	0.7224	22.75	2373	3.515	125.2
310	192.6	0.6691	21.43	2380	3.487	124.7
315	184.4	0.6584	20.92	2379	3.502	125
319	178.7	0.6177	19.75	2379	3.481	124.4
324	161.1	0.5546	17.74	2368	3.439	123.1
328	160.9	0.5482	17.6	2373	3.449	123.5
333	148.4	0.4762	15.43	2365	3.395	121.9

337	157.4	0.5255	16.86	2379	3.461	123.9
341	150.2	0.4938	15.94	2377	3.444	123.4
346	147.2	0.4658	15.03	2379	3.434	123.1
350	139.4	0.4433	14.41	2376	3.424	122.9
355	132.7	0.4026	13.22	2373	3.398	122.2
359	129	0.4022	13.03	2374	3.41	122.4

Table B.7. Time-dependent aerosol particle concentrations, volume concentrations, and surface area concentrations for *p*-ethyltoluene 1994 experiments.

NA, NB = particle number concentration not corrected for particle losses to walls (cm^{-3})
VA, VB = volume concentration not corrected for particle losses to walls ($\mu m^3\ cm^{-3}$)
SA, SB = surface area concentration not corrected for particle losses to walls ($\mu m^2\ cm^{-3}$)

NAcorr, NBcorr = particle number concentration corrected for particle losses (cm^{-3})
VAcorr, VBcorr = volume concentration corrected for particle losses ($\mu m^3\ cm^{-3}$)
SAcorr, SBcorr = surface area concentration corrected for particle losses ($\mu m^2\ cm^{-3}$)

8/29/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
1	1672	0.3208	22.42	1678	0.3218	22.49
5	1629	0.3081	21.63	1659	0.3133	21.97
10	1569	0.2792	20.17	1627	0.2889	20.83
14	1543	0.2628	19.33	1624	0.2758	20.23
18	1482	0.2671	19.05	1585	0.2836	20.19
23	1455	0.2539	18.44	1584	0.2746	19.86
27	1425	0.2444	17.94	1575	0.2682	19.58
32	1392	0.2377	17.35	1567	0.2654	19.26
36	1439	0.2545	18.37	1635	0.2855	20.51
41	1502	0.2534	18.65	1725	0.2887	21.08
45	1547	0.2506	18.8	1793	0.289	21.47
50	1508	0.246	18.54	1781	0.2882	21.49
54	1482	0.2423	18.2	1777	0.2876	21.38
59	1449	0.2442	18.01	1770	0.2934	21.46
63	1455	0.2428	18.08	1797	0.2951	21.76
68	1430	0.236	17.64	1797	0.2921	21.58
72	1420	0.2427	18	1807	0.3018	22.16
76	1358	0.2195	16.64	1765	0.2813	21.01
81	1401	0.2337	17.53	1832	0.2992	22.16
86	1332	0.2326	17.05	1787	0.3018	21.94
91	1352	0.2368	17.35	1831	0.3097	22.5
95	1312	0.2227	16.48	1809	0.2985	21.84
100	1286	0.233	16.84	1806	0.3127	22.46

104	1281	0.2183	16.39	1818	0.3005	22.21
109	1280	0.2138	16.08	1839	0.2994	22.14
113	1226	0.2197	16.04	1803	0.3082	22.3
117	1229	0.2199	16.16	1822	0.3111	22.61
122	1249	0.2333	16.93	1864	0.3281	23.64
126	1230	0.2145	16.09	1861	0.3118	22.99
131	1196	0.2189	16.07	1846	0.3197	23.2
135	1204	0.2148	16.09	1870	0.3182	23.41
140	1156	0.2192	15.92	1842	0.326	23.48
144	1152	0.2255	16.21	1852	0.3351	23.96
149	1142	0.2279	16.41	1861	0.341	24.4
153	1116	0.2171	15.79	1848	0.3328	23.97
157	1121	0.2342	16.6	1868	0.3529	24.97
162	1550	0.3205	22.9	2320	0.4441	31.61
166	1563	0.331	23.5	2353	0.4587	32.48
171	1532	0.3317	23.4	2344	0.4646	32.73
175	1514	0.342	23.9	2344	0.4791	33.51
180	1526	0.357	24.78	2379	0.4996	34.74
184	1483	0.3478	24.43	2353	0.4947	34.67
189	1483	0.3685	25.38	2374	0.5209	35.98
193	1469	0.3874	26.19	2376	0.5445	37.09
201	1439	0.4187	27.6	2377	0.5863	39.13
206	1399	0.4204	27.71	2356	0.5943	39.63
210	1408	0.4642	29.76	2380	0.6438	42.02
215	1373	0.4868	30.77	2363	0.6737	43.46
219	1372	0.5347	32.84	2376	0.7282	45.9
223	1349	0.5646	34.18	2367	0.765	47.63
228	1302	0.608	35.6	2337	0.8178	49.56
232	1302	0.6857	38.76	2351	0.9043	53.19
237	1301	0.7352	40.97	2367	0.9654	56
241	1257	0.7813	42.24	2337	1.022	57.78
246	1235	0.8585	44.96	2333	1.113	61.2
250	1240	0.9751	49.18	2352	1.243	66.07
254	1211	1.077	52.42	2338	1.361	70.01
259	1190	1.209	56.54	2336	1.515	75.14
263	1182	1.335	60.47	2344	1.663	79.98
268	1164	1.418	62.76	2347	1.775	83.48
272	1127	1.529	65.28	2328	1.912	87.07
277	1105	1.676	68.92	2329	2.098	92.23
281	1153	1.881	75.28	2400	2.34	100
285	1154	1.963	76.43	2425	2.461	102.6
290	1201	2.145	80.84	2507	2.702	109.2
294	1247	2.29	83.77	2583	2.9	114
299	1315	2.41	86.32	2692	3.095	119.2
303	1416	2.505	88.96	2828	3.255	124.1
308	1451	2.484	87.25	2908	3.317	125.2
312	1564	2.527	88.21	3060	3.432	128.6
317	1642	2.415	84.63	3187	3.408	127.9

321	1761	2.35	83.57	3346	3.411	129.2
326	1823	2.204	79.7	3458	3.347	128
330	1879	2.08	77.1	3551	3.284	127.5
334	1878	1.771	69.47	3585	3.024	121.6
339	1937	1.548	65.14	3684	2.851	119
345	1973	1.447	64.68	3766	2.799	120.4
349	1994	1.439	66.76	3815	2.819	123.6
353	2247	1.562	74.28	4101	2.971	132.4
358	2330	1.615	78.46	4223	3.058	138
362	2292	1.705	82.28	4215	3.176	143.1
367	2320	1.853	88.16	4281	3.36	150.6
371	2269	1.996	92.84	4262	3.536	156.7
376	2242	2.087	95.89	4273	3.67	161.5
380	2248	2.267	101.8	4310	3.887	169.1
385	2215	2.484	108.6	4318	4.159	178.1
389	2221	2.681	115.1	4356	4.404	186.6
393	2163	2.771	116.8	4331	4.545	190.3
398	2135	2.924	121	4346	4.768	197.2
402	2067	3.042	123.7	4311	4.945	202.1
407	2055	3.167	126.7	4343	5.15	208.2
411	1968	3.166	125.3	4290	5.215	209.3
416	1970	3.429	132.6	4337	5.57	220
420	1913	3.452	132.3	4316	5.67	222.4
424	1864	3.568	134.3	4303	5.867	227.4
429	1790	3.544	131.9	4273	5.947	228.6
433	1770	3.618	133.7	4289	6.107	233.5
438	1770	3.622	133.3	4335	6.22	236.9
442	1734	3.584	131.3	4336	6.268	237.9
447	1684	3.558	129.5	4331	6.351	239.9
451	1640	3.512	127.1	4322	6.392	240.6
455	1581	3.446	124.1	4297	6.413	240.6
460	1570	3.455	124.2	4329	6.531	244.4
464	1572	3.485	125	4366	6.65	248.2
469	1512	3.371	120.7	4348	6.643	247.6
473	1495	3.374	120.2	4364	6.732	250.1

9/2/94						
Time(min)	**NA**	**VA**	**SA**	**NAcorr**	**VAcorr**	**SAcorr**
1	698.9	0.1651	10.97	701.3	0.1656	11
10	690	0.1357	8.962	716.7	0.1414	9.288
23	479.7	0.1001	6.696	531.7	0.1107	7.326
32	451.2	9.56E-02	6.419	518.3	0.1092	7.239
41	456.5	0.1183	6.974	538.4	0.1356	7.998
50	1094	2.903	90.14	1216	3.022	94.39
63	485.5	0.128	8.123	631.7	0.2676	13.13
72	431.7	9.19E-02	6.116	591.1	0.2345	11.3
81	389.9	7.47E-02	5.294	562	0.2196	10.63

94	373.5	8.38E-02	5.499	562.2	0.2328	11.07
103	375.4	7.89E-02	5.36	576	0.2312	11.11
112	388.4	0.1012	6.237	603.8	0.2575	12.23
130	375.9	8.29E-02	5.647	614.2	0.2446	11.97
139	373.2	9.31E-02	6.059	622.3	0.2577	12.56
152	375.5	0.1109	6.87	638.5	0.2795	13.61
161	356.7	0.109	6.875	629	0.2814	13.82
170	365.6	0.1171	7.362	648.4	0.2942	14.54
183	427.3	0.2272	12	725.4	0.4109	19.53
192	331	0.1593	9.038	637	0.3476	16.81
201	340.2	0.1992	10.68	655.4	0.3932	18.73
213	452.6	0.3935	19.19	781.4	0.6007	27.86
222	354.3	0.3604	16.5	693.1	0.5794	25.68
231	428	0.4745	20	780.8	0.7114	29.91
244	486.4	0.6706	25.28	874.5	0.9482	36.7
253	1331	0.7743	28.99	1813	1.093	41.93
262	4321	0.821	39.41	5079	1.192	54.49
271	1.05E+04	1.163	82.74	1.19E+04	1.587	100.9
284	2.19E+04	3.272	251.9	2.45E+04	3.801	278
293	2.76E+04	6.379	436	3.11E+04	7.057	472.5
302	3.08E+04	10.37	636.1	3.52E+04	11.3	687.9
311	3.23E+04	15.06	845.3	3.77E+04	16.39	918.8
321	3.27E+04	20.49	1056	3.91E+04	22.49	1163
334	3.25E+04	28.01	1321	4.02E+04	31.29	1485
347	3.17E+04	36.21	1578	4.09E+04	41.37	1820

9/10/94						
Time(min)	**NA**	**VA**	**SA**	**NAcorr**	**VAcorr**	**SAcorr**
1	2400	0.3863	27.03	2410	0.388	27.13
5	1938	0.305	22.16	1978	0.3113	22.57
10	1876	0.2642	20.62	1953	0.2748	21.35
14	1884	0.3699	23.55	1993	0.3874	24.65
19	1797	0.2706	20.38	1940	0.293	21.81
23	1796	0.2573	19.7	1966	0.2833	21.39
28	1748	0.2439	19.05	1952	0.2741	21.04
32	1640	0.27	19.2	1869	0.3047	21.46
41	1621	0.2676	18.89	1906	0.3111	21.73
50	1655	0.2931	19.94	2000	0.3461	23.38
63	3558	10.39	314.1	4074	10.84	329.9
72	1585	0.2362	17.9	2155	0.69	34.23
81	1600	0.2306	17.94	2232	0.7276	35.92
93	1520	0.2252	17.46	2218	0.7313	36.1
102	1494	0.2519	18.4	2241	0.7653	37.56
111	1476	0.3714	21.7	2271	0.8983	41.55
120	1576	0.4209	23.86	2420	0.9622	44.45
133	1601	0.3633	23.19	2514	0.9169	44.58
142	1419	0.3044	20.78	2373	0.8664	42.72

151	1425	0.2926	21.15	2417	0.8633	43.66
160	1438	0.4023	25.36	2469	0.9851	48.55
173	1424	0.4171	27.44	2506	1.016	51.61
182	1395	0.5064	31.35	2523	1.118	56.31
191	1413	0.6272	36.99	2575	1.256	62.86
200	1368	0.8099	43.8	2571	1.462	70.86
211	1350	1.086	54.03	2605	1.778	82.98
220	1391	1.387	64.15	2691	2.125	95.13
233	2243	1.986	81.85	3712	2.83	117.2
242	4778	2.493	101.9	6587	3.452	141.8
251	1.01E+04	3.118	138.3	1.25E+04	4.237	184.8
260	1.78E+04	4	209.6	2.11E+04	5.335	265.5
273	2.83E+04	6.016	383.7	3.33E+04	7.699	457.1
282	3.29E+04	8.27	537.9	3.90E+04	10.21	626
291	3.57E+04	12	735.4	4.29E+04	14.27	842.2
299	3.68E+04	16.18	924.3	4.50E+04	18.83	1052
313	3.68E+04	23.38	1209	4.65E+04	27.02	1387
323	3.63E+04	29.74	1433	4.72E+04	34.45	1659
332	3.55E+04	34.22	1574	4.74E+04	40.11	1851
341	3.46E+04	38.12	1685	4.75E+04	45.45	2023

10/10/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
1	3425	0.4668	37.88	3438	0.4682	37.99
10	3436	0.4636	37.73	3564	0.4773	38.86
23	3877	0.5371	43.32	4175	0.5693	45.97
32	3912	0.5333	43.56	4342	0.58	47.4
41	3879	0.5386	43.32	4438	0.5995	48.33
50	3843	0.5306	42.9	4530	0.6059	49.07
59	3723	0.5169	41.86	4534	0.6061	49.17
72	3656	0.5091	41.15	4639	0.6179	50.06
83	3517	0.5083	40.61	4641	0.6333	50.83
92	3402	0.4746	38.53	4637	0.6124	49.8
101	3361	0.4922	39.03	4706	0.6431	51.35
110	3272	0.473	37.93	4721	0.6365	51.26
119	3207	0.4719	37.66	4759	0.6479	52
132	3138	0.4743	37.68	4833	0.6685	53.46
141	3029	0.4566	36.29	4819	0.6629	53.03
150	2953	0.4656	36.46	4834	0.684	54.16
159	2879	0.4588	35.97	4848	0.6893	54.61
173	2817	0.4639	36.11	4918	0.7132	56.22
182	2821	0.4896	37.66	5002	0.7514	58.72
191	3422	0.6189	47.02	5692	0.8952	69.17
201	3339	0.6196	46.98	5712	0.9137	70.46
210	3332	0.6652	49.5	5794	0.9763	74.21
219	3230	0.7035	51.07	5778	1.033	77.06
233	3167	0.8029	56.01	5839	1.163	84.09

242	3131	0.8963	60.53	5879	1.279	90.08
250	3126	1.037	67.33	5939	1.442	98.31
259	3068	1.205	74.81	5952	1.641	107.6
273	2975	1.54	88.58	5969	2.036	124.6
282	2954	1.943	103.8	6021	2.492	142.5
291	2828	2.342	117	5970	2.96	159.1
299	2838	2.799	132.6	6051	3.495	178.2
314	2632	3.459	149.7	5989	4.346	203.4
325	2568	4.182	168.2	6049	5.272	229.9
334	2434	4.588	174.8	6023	5.885	244.3
343	2411	5.076	185.5	6117	6.623	263.9
352	2517	5.672	201	6355	7.532	290.3
361	2434	5.916	203.3	6406	8.125	304.5

11/1/94						
Time(min)	**NA**	**VA**	**SA**	**NAcorr**	**VAcorr**	**SAcorr**
1	991.9	0.1526	11.61	995.7	0.1531	11.64
10	956.2	0.1422	10.9	993.7	0.1469	11.25
23	937.7	0.1316	10.43	1021	0.1416	11.19
32	899.5	0.1358	10.46	1013	0.1495	11.51
41	900.5	0.1289	10.18	1045	0.1462	11.5
50	904.9	0.1346	10.46	1080	0.1556	12.08
63	932.1	0.1335	10.61	1152	0.16	12.65
72	929.9	0.1397	10.8	1181	0.1699	13.13
85	911.1	0.1482	11.26	1204	0.1842	14.02
94	887.1	0.134	10.51	1208	0.1738	13.57
103	926.2	0.1519	11.33	1277	0.1958	14.68
112	880	0.1432	10.94	1259	0.191	14.59
121	874.5	0.1436	10.87	1281	0.1952	14.81
130	917.7	0.153	11.49	1352	0.2089	15.74
143	860.3	0.1458	11.06	1334	0.208	15.76
152	889.6	0.1544	11.64	1390	0.2205	16.63
161	842.6	0.1473	11.1	1368	0.2177	16.39
170	789.5	0.1487	10.93	1338	0.2231	16.51
179	777.1	0.1462	10.87	1349	0.2245	16.74
192	743.1	0.1482	10.76	1345	0.2326	17.05
203	729.5	0.1598	11.19	1356	0.2495	17.83
212	749.4	0.3011	15.41	1397	0.4006	22.5
221	689.2	0.1662	11.43	1355	0.2702	18.82
230	637.8	0.1561	10.8	1321	0.2646	18.48
243	700.4	0.1972	13.09	1409	0.3132	21.24
252	648.9	0.2026	13.11	1373	0.3239	21.58
261	627.1	0.2149	13.62	1366	0.3419	22.44
270	631.1	0.229	14.34	1385	0.3624	23.52
283	609.7	0.2675	15.92	1384	0.4114	25.69
292	609.3	0.3032	17.4	1398	0.4559	27.62
301	595.9	0.3469	19.03	1400	0.5092	29.76

312	591.6	0.4042	21.14	1413	0.5811	32.58
321	570.8	0.4453	22.46	1408	0.6359	34.55
330	573.5	0.5278	25.28	1426	0.7354	38.13
343	547.4	0.6064	27.58	1424	0.8431	41.71
352	544.8	0.6821	29.84	1440	0.9475	45.13
361	528.1	0.7489	31.55	1441	1.042	47.97
370	514.4	0.832	33.68	1446	1.159	51.43

Table B.8. Time-dependent aerosol particle concentrations, volume concentrations, and surface area concentrations for 1,2,4-trimethylbenzene 1994 experiments.

NA, NB = particle number concentration not corrected for particle losses to walls (cm^{-3})
VA, VB = volume concentration not corrected for particle losses to walls ($\mu m^3\ cm^{-3}$)
SA, SB = surface area concentration not corrected for particle losses to walls ($\mu m^2\ cm^{-3}$)

NAcorr, NBcorr = particle number concentration corrected for particle losses (cm^{-3})
VAcorr, VBcorr = volume concentration corrected for particle losses ($\mu m^3\ cm^{-3}$)
SAcorr, SBcorr = surface area concentration corrected for particle losses ($\mu m^2\ cm^{-3}$)

8/27/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
0	5224	1.05	72.96	5224	1.05	72.96
12	4614	0.8921	62.59	4825	0.9305	65.11
21	4292	0.7964	56.76	4646	0.8587	60.91
30	4207	0.7529	54.31	4698	0.8377	60
39	4033	0.7242	52.21	4656	0.8304	59.38
53	3956	0.7213	52.21	4757	0.8556	61.35
61	3949	0.7409	53.68	4839	0.8915	63.93
70	3968	0.8519	59.52	4974	1.026	71.33
83	4040	1.047	70.9	5198	1.261	85.26
92	2722	0.3251	18.65	4075	0.5616	34.39
110	1982	1.784	86.79	3784	2.097	106.4
119	4450	5.61	241	6402	6.102	268.3
128	5855	9.202	339.4	8079	10.1	381.5
137	8204	11.04	396.4	1.08E+04	12.6	461.1
146	1.01E+04	8.785	364.1	1.31E+04	10.92	448.9
155	1.14E+04	9.056	425.8	1.48E+04	11.54	525.3
164	1.19E+04	14.42	613	1.57E+04	17.43	733.9
174	5147	10.04	372.8	9132	13.48	509.3
183	1.37E+04	29.46	1074	1.84E+04	34.46	1265
192	1.29E+04	30.76	1089	1.81E+04	37.52	1340

9/4/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
0	3522	0.7756	52.14	3522	0.7756	52.14
5	3456	0.7579	50.63	3518	0.7706	51.43
9	3400	0.7375	49.67	3511	0.76	51.09
14	3169	0.696	46.48	3337	0.7301	48.63
18	3043	0.6208	42.62	3255	0.6632	45.31
22	2973	0.5988	41.22	3228	0.649	44.43
27	2908	0.5893	40.44	3216	0.6494	44.28
31	2866	0.5661	39.35	3215	0.6336	43.68
40	2834	0.5464	38.43	3273	0.6299	43.83
49	2722	0.5363	37.74	3248	0.6353	44.19
63	2744	0.6217	42.43	3393	0.7464	50.57
71	2809	0.7762	51.17	3524	0.9192	60.45
80	2871	1.15	69.08	3655	1.322	80.01
95	2956	2.8	132.9	3874	3.104	149.9
104	3976	5.636	224.4	5062	6.148	249.5
112	1.04E+04	8.681	325.4	1.20E+04	9.591	364.8
121	2.34E+04	9.065	465.6	2.58E+04	10.49	524.8
130	3.34E+04	18.4	968.2	3.67E+04	20.31	1051
139	3.72E+04	38.56	1707	4.17E+04	41.65	1841
153	3.72E+04	63.27	2449	4.38E+04	70.44	2736
161	3.53E+04	73.1	2689	4.34E+04	83.68	3095
170	3.49E+04	81.81	2912	4.47E+04	96.9	3473
179	3.64E+04	90.9	3186	4.81E+04	111.4	3931
184	3.49E+04	89.94	3128	4.77E+04	113.5	3975
188	3.37E+04	88.06	3052	4.73E+04	114	3979
192	3.27E+04	86.65	2994	4.71E+04	115	4000
197	3.16E+04	84.9	2922	4.70E+04	116.1	4026
201	3.05E+04	82.7	2840	4.67E+04	116.2	4019
207	2.88E+04	78.93	2702	4.60E+04	115.8	3991
211	2.75E+04	76.27	2605	4.55E+04	115.2	3965
216	2.64E+04	73.63	2512	4.52E+04	115.2	3957
220	2.54E+04	71.25	2428	4.49E+04	114.8	3939
225	2.47E+04	69.37	2364	4.50E+04	115.4	3956
229	2.35E+04	66.19	2255	4.44E+04	114	3908
233	2.24E+04	63.26	2153	4.39E+04	112.9	3865
238	2.14E+04	60.83	2068	4.36E+04	112.6	3851
242	2.05E+04	57.98	1973	4.32E+04	111.4	3810
247	1.96E+04	55.36	1885	4.29E+04	110.7	3786
251	1.87E+04	52.99	1805	4.25E+04	109.8	3755
256	1.78E+04	50.23	1714	4.22E+04	108.8	3722
260	1.69E+04	47.99	1635	4.18E+04	107.9	3688
264	1.63E+04	46.21	1576	4.16E+04	107.4	3671
269	1.55E+04	43.73	1492	4.12E+04	106.5	3638
273	1.49E+04	42.03	1435	4.10E+04	106	3619
278	1.43E+04	40.21	1375	4.09E+04	105.5	3606
282	1.37E+04	38.54	1317	4.06E+04	104.9	3584

9/16/94 Time(min)	NB	VB	SB	NBcorr	VBcorr	SBcorr
0	2190	0.2822	23.08	2190	0.2822	23.08
5	2154	0.2815	22.9	2195	0.2858	23.25
9	2159	0.2823	22.98	2232	0.2901	23.61
14	2117	0.2678	22.18	2231	0.2796	23.15
18	2087	0.2752	22.36	2232	0.2904	23.62
22	2088	0.2703	22.28	2264	0.2888	23.8
27	2057	0.2678	22.13	2271	0.2902	23.98
31	2005	0.2611	21.35	2249	0.2867	23.47
40	1950	0.2556	21.02	2260	0.2882	23.72
49	1893	0.2539	20.67	2267	0.2935	23.94
62	1849	0.252	20.53	2312	0.3015	24.61
71	1810	0.26	20.82	2332	0.3167	25.46
80	1858	0.2813	22.26	2437	0.3451	27.47
93	1824	0.3108	23.96	2476	0.3858	30.03
101	1865	0.3665	27.4	2562	0.4495	34.06
110	1847	0.4742	32.98	2589	0.5687	40.42
119	1872	0.6517	41.93	2659	0.7616	50.33
133	1905	1.241	66.69	2762	1.395	77.43
141	1965	1.96	92.15	2872	2.163	105.2
150	2201	3.094	126.1	3194	3.407	143.6
159	2810	4.471	164	3933	4.993	189
173	3897	5.037	184.7	5292	6.068	226.9
181	4824	4.361	189.9	6366	5.606	239.8
190	5715	5.732	254.9	7442	7.187	313.6
201	5829	7.81	322.7	7804	9.637	396.1
210	5832	9.701	378.6	8033	11.95	467.9
219	5734	11.77	433.6	8189	14.6	543.8
232	5060	12.95	450.6	7909	16.85	597.4
241	4754	12.89	442.3	7877	17.6	616
246	4496	12.58	428.2	7764	17.73	616.4
250	4200	12.02	407.1	7579	17.52	606.6
255	4151	11.93	403.6	7667	17.85	617
259	3945	11.47	387.1	7566	17.72	611.3
263	3826	11.16	376.4	7549	17.73	611
268	3647	10.68	359.8	7493	17.63	607
272	3607	10.61	357.4	7549	17.86	614.5
277	3412	10.12	340.4	7470	17.74	609.5
281	3335	9.91	333.2	7484	17.81	611.6
286	3143	9.306	313.1	7398	17.54	602.5
290	3126	9.276	312.1	7466	17.78	610.2
294	3066	9.132	307	7490	17.9	613.8
299	2950	8.752	294.6	7473	17.83	611.6
303	2679	7.974	268.4	7275	17.28	592.9
308	2565	7.601	256.4	7248	17.18	589.8
314	2491	7.401	249.6	7274	17.3	593.3

318	2456	7.234	244.6	7306	17.33	595.1
323	2414	7.2	242.4	7345	17.56	601.3
327	2317	6.844	231.2	7311	17.39	596.5
331	2244	6.566	222.4	7298	17.3	593.9
336	2238	6.576	222.6	7366	17.54	601.7
340	2128	6.219	211	7313	17.36	595.9
345	2066	6.075	205.7	7320	17.43	597.6
349	2056	6.048	204.8	7365	17.57	602.2
353	2001	5.865	198.7	7364	17.55	601.7
358	1926	5.69	192.4	7354	17.58	601.9
362	1870	5.507	186.6	7347	17.55	601.2
367	1824	5.348	181.4	7362	17.58	602.2
371	1811	5.322	180.5	7398	17.7	606.2
375	1763	5.198	176.1	7397	17.73	606.6
380	1691	4.932	167.6	7381	17.63	603.8
384	1647	4.819	163.7	7381	17.65	604.4
389	1602	4.683	159.1	7389	17.68	605.2
393	1573	4.622	156.9	7402	17.75	607.2

9/21/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
0	1673	0.1966	16.28	1673	0.1966	16.28
5	1488	0.1793	14.78	1517	0.1821	15.02
9	1529	0.1797	14.86	1583	0.1849	15.28
14	1407	0.1578	13.44	1489	0.1654	14.08
18	1444	0.1595	13.49	1549	0.1691	14.31
22	1400	0.1521	13.06	1527	0.1638	14.04
27	1328	0.1431	12.39	1483	0.1569	13.57
31	1353	0.1466	12.58	1529	0.1624	13.92
40	1284	0.1422	12.2	1506	0.1621	13.9
54	1228	0.142	11.99	1518	0.1682	14.23
63	1242	0.1418	12.21	1574	0.172	14.79
72	1211	0.1503	12.76	1582	0.1844	15.68
84	1325	0.1944	15.81	1746	0.2348	19.24
93	1407	0.2417	18.99	1865	0.2881	22.89
102	1357	0.1653	13	1892	0.2173	17.34
111	1132	0.3981	25.1	1729	0.4606	30.11
124	1438	0.8143	45.8	2083	0.9033	52.27
133	1462	1.321	64.46	2146	1.447	72.67
142	1508	2.007	86.01	2245	2.198	97.02
151	1900	2.988	113.4	2727	3.308	129.2
160	2931	4.239	150.9	3906	4.793	174.8
173	4150	3.331	141	5367	4.236	177.1
182	4747	3.445	165.9	6113	4.48	207.5
192	5283	6.286	267.5	6841	7.564	319.1
201	5403	9.114	351.5	7170	10.78	417.7
210	5187	10.99	399	7195	13.24	485.3

215	5057	11.48	409.4	7205	14.1	508.5
219	3100	6.627	240.3	5314	9.411	345.2
224	960.8	1.819	68.98	3200	4.653	175.6
232	3166	8.62	295.5	5564	11.93	418
236	3840	10.57	361	6337	14.18	493.3
241	3687	10.13	346.2	6302	14.1	490.3
245	3501	9.654	329.9	6205	13.89	483
250	3306	9.128	312.4	6116	13.68	476
254	2447	7.081	239.3	5322	11.84	409.6
258	3012	8.463	288.8	5965	13.46	466.9
263	2902	8.136	278.3	5948	13.41	465.7
267	2701	7.494	257.3	5816	12.98	451.6
272	1626	4.82	162.6	4797	10.48	362.6
276	1359	3.59	125	4563	9.341	328.2
281	2369	6.557	225.8	5648	12.53	436.5
285	1470	3.72	131.8	4783	9.788	345.7
289	1413	3.718	130.7	4761	9.881	347.8
294	1953	5.74	195.3	5365	12.1	419
298	2150	6.004	207.2	5617	12.52	436.2
303	2070	5.733	198.4	5603	12.44	433.8
307	1649	4.862	165	5226	11.7	404.8
311	1973	5.502	190.1	5600	12.49	434.8
316	1909	5.382	185.7	5597	12.55	436.4
320	1839	5.241	180.3	5575	12.54	435.7
325	1802	5.107	175.9	5596	12.58	437
329	1754	4.932	170.3	5592	12.53	435.7
334	1729	4.833	167.2	5622	12.59	438
338	1686	4.739	163.8	5622	12.62	438.8
345	1601	4.502	155.6	5608	12.59	437.5
350	1579	4.45	153.8	5636	12.68	440.6
354	1596	4.565	157	5695	12.91	447.8
359	1494	4.214	145.7	5641	12.7	441.2
363	1482	4.211	145.2	5667	12.81	444.4
367	1065	2.977	103.4	5277	11.65	405.2
372	1393	3.916	135.5	5649	12.72	441.6
376	1343	3.815	131.6	5633	12.71	441.1
381	1303	3.672	127	5635	12.69	440.5
385	1287	3.615	125.2	5652	12.72	441.8
389	1256	3.528	122.1	5653	12.73	441.8

10/6/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
0	2069	0.2316	19.49	2069	0.2316	19.49
4	1960	0.2342	19.02	1993	0.2372	19.27
9	1987	0.2187	18.49	2063	0.2252	19.04
13	1965	0.2209	18.38	2075	0.2303	19.17
18	1902	0.2138	17.84	2052	0.2268	18.92

22	1898	0.2148	17.82	2080	0.2305	19.14
27	1867	0.2075	17.37	2089	0.2267	18.97
31	1815	0.1899	16.47	2067	0.2115	18.29
40	1796	0.1896	16.29	2117	0.2168	18.6
49	1745	0.1866	15.99	2133	0.2193	18.77
62	1645	0.1791	15.43	2125	0.2193	18.86
71	1588	0.1789	15.1	2128	0.2243	18.98
83	1566	0.1815	15.41	2181	0.2336	19.87
92	1553	0.19	16	2221	0.2475	20.9
101	1570	0.2279	18.35	2285	0.2911	23.72
110	1558	0.2545	19.98	2318	0.3243	25.86
123	1580	0.3508	25.49	2399	0.4327	32.23
132	1566	0.4343	29.9	2423	0.5266	37.34
141	1550	0.5737	36.43	2443	0.6791	44.69
150	1531	0.8184	46.55	2460	0.9438	55.9
163	1458	1.232	61.3	2441	1.403	72.91
172	1402	2.009	84.93	2431	2.245	99.26
181	1314	2.52	97.24	2399	2.869	115.8
190	1261	2.869	103.6	2409	3.36	127.3
201	1637	3.243	108.4	2916	3.99	140.6
210	2747	2.062	77.58	4178	2.976	115.3
223	5902	1.827	104.5	7625	2.855	147.2
232	8039	3.677	198.2	1.00E+04	4.81	246.2
241	9257	6.7	324	1.15E+04	8.033	381.1
250	9657	10.34	450.2	1.22E+04	12.05	522.7
259	9663	14.37	573.2	1.26E+04	16.72	669.7
272	8651	17.82	652.7	1.21E+04	21.47	795.4
281	7595	17.61	626.6	1.15E+04	22.29	804.3
286	7002	17.07	600.3	1.11E+04	22.31	797.2
290	6597	16.52	577	1.08E+04	22.21	788.9
294	6288	16	557.5	1.07E+04	22.13	783.9
299	5839	15.13	524.8	1.04E+04	21.77	768.6
308	5009	13.16	456	9845	20.61	726.7
312	4562	12.16	420.7	9511	19.94	702.5
317	4224	11.27	390.1	9304	19.43	684.7
321	3919	10.4	361.3	9096	18.85	665.3
326	3690	9.766	339.7	8980	18.54	654.6
330	3477	9.233	321.1	8852	18.25	644.3
335	3173	8.389	292.6	8645	17.68	625.2
339	2990	7.992	278.3	8536	17.5	618
343	2824	7.592	264.1	8440	17.3	610.5

10/16/94 Side A

Time(min)	NA	VA	SA	NAcorr	VAcorr	SAcorr
1	3589	0.5183	39.89	3604	0.52	40.02
10	3364	0.4578	36.36	3501	0.4727	37.53
23	3119	0.4298	33.96	3425	0.4633	36.57

32	2954	0.406	32.17	3370	0.452	35.73
41	2945	0.4325	33.82	3463	0.49	38.3
50	2257	0.3325	25.81	2863	0.4006	31.07
62	2165	0.325	25.36	2877	0.4059	31.6
71	2084	0.3787	27.34	2865	0.4691	34.28
80	1976	0.362	26.23	2823	0.4627	33.88
93	2127	0.4582	32.53	3068	0.581	41.52
102	2186	0.5763	38.61	3189	0.7143	48.55
111	2158	0.7497	46.71	3223	0.9071	57.81
124	2292	1.182	66.02	3461	1.382	79.41
133	2243	1.587	81.57	3478	1.831	97.12
142	2261	2.12	99.07	3570	2.429	117.6
151	1757	2.307	97.41	3142	2.701	119.4
160	1646	2.935	113	3103	3.451	139.7
170	1513	3.468	122.4	3065	4.185	156.1
179	1309	3.411	114.9	2983	4.343	155.8
184	1197	3.141	104.8	2914	4.19	149.5
188	1069	2.715	90.86	2818	3.846	138.2
193	939.9	2.18	74.38	2722	3.39	124.3
197	851.9	1.706	60.04	2658	2.963	111.5
201	816.7	1.431	52.28	2644	2.725	105
206	869	1.249	48.18	2721	2.578	102.2
210	741.7	1.178	44.65	2612	2.533	99.64
215	710.8	1.135	43.14	2603	2.522	99.27
219	773.3	1.389	51.29	2683	2.806	108.6
224	651.8	1.085	40.34	2582	2.533	98.71
228	653.1	1.139	41.88	2599	2.615	101.2
233	611	1.118	40.52	2576	2.627	101
237	625.4	1.171	42.09	2606	2.709	103.6
242	628.1	1.111	39.99	2628	2.685	102.8
246	636.5	1.141	40.73	2652	2.744	104.5
251	624.3	1.12	39.82	2659	2.76	104.9
255	587.5	1.031	36.95	2637	2.698	102.9
259	577.6	1.061	37.55	2641	2.756	104.5
264	580.2	1.039	37.07	2661	2.769	105.2
268	624.3	1.023	36.77	2720	2.781	105.8
273	569.2	1.087	38.13	2682	2.883	108.5
277	531.1	0.98	34.66	2657	2.803	105.9
282	693.4	1.022	36.22	2844	2.88	108.7
286	518.4	0.9768	34.56	2681	2.862	107.9
291	502.1	0.9596	34.03	2680	2.878	108.5
295	584.6	0.9729	35.12	2775	2.918	110.5
299	641.2	0.9693	34.44	2850	2.942	110.7

10/16/94 Side B

Time(min)	NB	VB	SB	NBcorr	VBcorr	SBcorr
1	1765	0.2585	20.04	1771	0.2593	20.1
5	1746	0.2469	19.53	1779	0.2507	19.83
10	1663	0.2262	18.26	1728	0.2333	18.83
14	1697	0.237	18.89	1788	0.247	19.7
19	1646	0.2281	18.27	1768	0.2414	19.35
23	1632	0.227	18.09	1779	0.2431	19.39
27	1610	0.2305	18.12	1781	0.2494	19.64
32	1576	0.218	17.54	1776	0.2401	19.33
36	1526	0.2196	17.45	1750	0.2444	19.44
41	1476	0.2184	17.01	1727	0.2467	19.27
45	1576	0.2278	17.97	1850	0.2588	20.45
50	1683	0.2513	19.59	1987	0.2862	22.37
58	1682	0.2589	19.97	2036	0.3003	23.23
62	1675	0.2651	20.26	2052	0.3099	23.77
71	1603	0.2645	20.39	2030	0.3163	24.43
80	1623	0.3144	23.12	2097	0.3742	27.75
93	1634	0.4152	28.7	2170	0.4894	34.3
102	1704	0.5946	37.93	2280	0.6829	44.39
111	1728	0.8759	50.37	2344	0.9856	58.02
120	1691	1.238	63.94	2349	1.381	73.23
133	1744	2.23	97.26	2479	2.467	110.6
142	1838	3.22	124.8	2651	3.585	143.1
151	2896	4.953	175.6	3866	5.571	202.9
160	4880	5.17	183.6	6107	6.12	222.1
170	8528	3.624	174.1	1.01E+04	4.847	222.6
179	1.13E+04	4.764	261.6	1.33E+04	6.142	317.6
193	1.40E+04	11.45	539.5	1.66E+04	13.31	617.8
201	1.45E+04	17.37	739.1	1.75E+04	19.82	840.7
210	1.44E+04	23.24	912.1	1.80E+04	26.72	1052
215	1.43E+04	25.92	984.5	1.82E+04	30.15	1152
219	1.38E+04	28.19	1038	1.80E+04	33.11	1229
224	1.33E+04	29.62	1067	1.78E+04	35.48	1290
228	1.29E+04	30.3	1076	1.77E+04	36.94	1326
233	1.23E+04	30.3	1064	1.75E+04	37.96	1348

10/18/94

Time(min)	NB	VB	SB	NBcorr	VBcorr	SBcorr
1	3026	0.3838	31.39	3038	0.385	31.49
5	2919	0.3495	29.27	2976	0.3551	29.74
10	2926	0.3515	29.54	3039	0.3624	30.47
14	2937	0.3523	29.6	3095	0.3676	30.89
19	2881	0.3524	29.29	3095	0.3731	31.04
23	2944	0.348	29.48	3204	0.373	31.6
28	2863	0.343	28.89	3178	0.3731	31.45
32	2825	0.3407	28.64	3184	0.375	31.55

37	2801	0.3389	28.48	3213	0.3784	31.83
41	2815	0.3458	28.99	3269	0.3895	32.7
46	2788	0.3493	28.86	3297	0.3984	33.01
50	2854	0.3571	29.7	3405	0.4106	34.22
55	2804	0.3506	29.25	3408	0.4093	34.22
59	2812	0.3529	29.42	3457	0.4159	34.75
73	2744	0.3444	28.83	3532	0.4223	35.4
91	2727	0.3969	32.01	3686	0.4947	40.22
100	2765	0.4272	34.09	3805	0.5359	43.16
113	2782	0.5412	40.63	3932	0.6687	51.11
122	2897	0.6843	48.9	4119	0.8282	60.53
131	2958	0.9423	62.19	4249	1.108	75.24
140	3468	1.394	86.29	4834	1.593	101.3
153	3455	2.245	120.7	4941	2.521	139.7
162	3384	3.168	152.8	4962	3.535	176.1
171	3352	4.401	191	5037	4.914	220.5
184	3197	6.774	252.1	5078	7.676	296.2
193	3173	8.031	278.4	5228	9.371	337.7
204	2994	8.048	266	5280	10.06	347

10/30/94						
Time(min)	**NB**	**VB**	**SB**	**NBcorr**	**VBcorr**	**SBcorr**
0	3493	0.458	36.7	3493	0.458	36.7
9	3284	0.4178	33.84	3402	0.4299	34.82
23	3131	0.3763	31.41	3429	0.405	33.79
32	3031	0.3702	30.82	3437	0.409	34.06
41	2968	0.3618	30.38	3478	0.4104	34.46
50	2878	0.3561	29.64	3490	0.4143	34.55
63	2810	0.3571	29.68	3563	0.4292	35.77
72	2824	0.3768	30.98	3668	0.4589	37.89
81	2769	0.3908	31.66	3701	0.4833	39.42
93	2735	0.446	35.05	3776	0.5541	44.02
102	2833	0.5429	41.1	3950	0.6644	51.06
111	2854	0.6512	46.94	4042	0.7886	58.02
120	2878	0.8217	55.58	4135	0.9793	67.97
129	2910	1.017	65.36	4234	1.199	79.3
142	2905	1.59	89.96	4327	1.827	106.9
151	2851	2.147	110.4	4346	2.443	130.2
160	2930	2.951	138.9	4506	3.334	162.8
173	3443	5.434	222.6	5171	6.052	256
182	3289	6.771	255.4	5159	7.685	299.9
191	3247	8.062	286.4	5281	9.387	345.3
206	2677	8.266	271.8	5002	10.5	360.5
211	2519	7.758	253.9	4936	10.29	352.2
215	2169	6.423	212.2	4647	9.157	316.8
220	1912	5.205	175.8	4453	8.132	286.7
224	1683	4.168	145.3	4264	7.211	260

228	1549	3.525	126.5	4164	6.658	244.4
233	1458	3.026	112.6	4111	6.246	233.5
237	1421	2.951	110.8	4103	6.235	234
242	1362	2.856	107.1	4078	6.215	233.1
246	1339	2.897	107.8	4083	6.32	236.1
251	1356	3.084	113.2	4137	6.591	244.6
255	1357	3.215	116.7	4167	6.795	250.7
260	1334	3.322	118.8	4183	7	256.2
264	1330	3.51	123.3	4212	7.273	263.7
268	1300	3.562	123.9	4213	7.414	267.3
273	1310	3.715	127.8	4266	7.687	275.3
277	1297	3.818	130	4287	7.89	280.9
282	1256	3.826	128.9	4289	8.029	284.2
286	1269	4.003	133.7	4338	8.316	292.7
291	1215	3.886	129.1	4328	8.335	292.6
295	1198	3.836	127.4	4345	8.393	294.4
299	1185	3.948	129.8	4367	8.619	300.5
304	1160	3.88	127.3	4385	8.691	302.6
308	1144	3.921	127.7	4404	8.848	306.8
313	1110	3.85	124.9	4413	8.921	308.7
317	1069	3.773	121.8	4406	8.957	309.2
322	1049	3.712	119.8	4427	9.037	311.7

APPENDIX C

Mass Spectral Library of Standards of Species Identified in Secondary Organic Aerosol

Table C.1. Mass spectral data of standards identified in SOA.

#1: BENZOIC ACID
Modified:scaled

Entry Number 1 from C:\DATABASE\hjf.l
CAS 000065-85-0
Melting Point -300
Boiling Point -300
Retention Index 69.239
Mol Formula C7H6O2
Mol Weight 122.037

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	57.00	39.95	57.00	54.95	40.00	66.05	156.00
27.00	240.00	40.90	8.00	56.00	3.00	67.00	16.00
28.90	24.00	41.95	10.00	57.00	5.00	67.95	7.00
30.90	5.00	44.90	112.00	58.00	1.00	70.05	2.00
32.85	5.00	46.90	120.00	59.05	1.00	71.00	2.00
34.40	0.00	47.90	14.00	59.95	25.00	71.95	12.00
34.90	2.00	48.90	133.00	60.95	75.00	72.90	136.00
35.90	27.00	49.90	1391.00	61.95	61.00	73.95	519.00
36.95	199.00	50.90	2774.00	62.95	90.00	74.95	280.00
37.95	380.00	52.05	461.00	64.00	31.00	76.05	528.00
38.90	483.00	54.00	8.00	65.00	207.00	77.05	6775.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
78.05	607.00	92.05	17.00	101.95	2.00	113.95	0.00
79.05	33.00	93.00	42.00	103.00	7.00	114.65	0.00
79.95	2.00	94.05	240.00	105.05	9999.00	115.00	1.00
81.05	2.00	95.05	18.00	106.05	785.00	115.80	0.00
82.10	3.00	96.05	3.00	107.05	50.00	115.90	0.00
82.95	2.00	96.90	1.00	108.00	2.00	116.05	0.00
85.05	5.00	97.05	2.00	109.00	0.00	116.55	0.00
86.95	5.00	98.00	0.00	110.00	2.00	116.85	1.00
88.95	2.00	99.00	1.00	111.00	1.00	118.10	1.00
89.95	2.00	99.20	1.00	112.20	1.00	119.05	6.00
91.05	7.00	100.95	3.00	113.00	0.00	120.00	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.05	9226.00	134.10	0.00	142.95	0.00	153.00	0.00

123.05	723.00	135.05	2.00	143.95	0.00	153.45	0.00
124.05	66.00	136.00	3.00	144.20	0.00	153.85	1.00
125.05	5.00	137.05	0.00	145.00	1.00	154.05	0.00
126.05	1.00	137.20	1.00	145.25	1.00	155.10	2.00
127.05	1.00	139.25	0.00	145.95	0.00	157.45	0.00
128.00	1.00	140.00	1.00	147.95	0.00	158.20	0.00
129.00	1.00	140.80	0.00	150.05	0.00	161.05	0.00
129.90	0.00	141.05	0.00	150.95	1.00	162.05	0.00
132.00	0.00	141.30	0.00	151.20	0.00	162.70	0.00
133.05	0.00	142.20	0.00	152.10	0.00	163.10	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
163.80	0.00	184.20	0.00	214.20	0.00		
165.05	1.00	185.30	0.00	220.05	1.00		
165.45	0.00	185.95	0.00				
167.70	0.00	186.20	0.00				
167.95	0.00	189.20	0.00				
169.00	1.00	190.70	0.00				
175.20	0.00	191.05	0.00				
180.05	0.00	192.95	0.00				
180.45	0.00	201.20	0.00				
180.95	1.00	207.00	1.00				
183.05	0.00	211.95	0.00				

#2: 2,4-PENTANEDIONE
Modified: scaled
Entry Number 2 from C:\DATABASE\hjf.l
CAS 000123-54-6
Melting Point -300
Boiling Point -300
Retention Index 28.149
Mol Formula C5H8O2
Mol Weight 100.052

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	127.00	36.90	59.00	49.95	32.00	60.95	10.00
27.05	485.00	37.95	108.00	50.90	28.00	62.00	9.00
28.90	431.00	39.00	441.00	51.95	11.00	62.95	7.00
29.95	18.00	39.90	74.00	52.95	86.00	63.90	3.00
30.90	260.00	40.95	523.00	54.00	17.00	64.95	4.00
32.85	3.00	41.95	570.00	55.00	169.00	65.95	11.00
33.40	0.00	43.05	9999.00	55.95	13.00	67.00	43.00
33.60	0.00	44.90	5.00	57.00	77.00	68.00	14.00
33.85	3.00	46.90	1.00	58.00	354.00	68.90	117.00
34.85	1.00	47.90	2.00	59.05	13.00	69.95	7.00
35.90	10.00	48.90	6.00	60.00	6.00	70.95	10.00
72.00	586.00	78.00	2.00	89.10	1.00	94.05	0.00
73.00	28.00	79.10	2.00	89.30	0.00	94.15	1.00

74.00	2.00	79.85	0.00	90.00	0.00	94.30	0.00
74.40	0.00	80.35	1.00	91.05	2.00	94.60	0.00
74.85	0.00	81.00	2.00	91.85	0.00	95.15	1.00
75.10	0.00	81.95	6.00	92.10	1.00	95.40	0.00
75.40	0.00	83.95	58.00	93.05	2.00	96.00	2.00
75.80	1.00	85.00	4528.00	93.55	0.00	97.95	1.00
76.05	1.00	86.00	198.00	93.65	0.00	98.05	2.00
76.15	0.00	87.00	22.00	93.80	0.00	98.15	0.00
76.95	3.00	87.95	2.00	93.90	1.00	98.35	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
100.00	3565.00	106.15	0.00	111.15	0.00	121.00	0.00
101.00	215.00	107.35	0.00	113.05	0.00	121.95	1.00
102.05	20.00	107.65	0.00	113.30	0.00	122.15	2.00
102.80	1.00	108.05	0.00	114.05	1.00	122.40	0.00
103.15	2.00	108.30	0.00	114.90	0.00	122.90	1.00
104.05	1.00	108.80	0.00	115.20	1.00	123.40	0.00
105.00	2.00	108.90	0.00	116.65	0.00	123.65	0.00
105.75	0.00	109.05	0.00	117.05	1.00	123.95	0.00
105.80	0.00	109.55	0.00	117.30	0.00	125.30	0.00
105.90	0.00	109.95	0.00	119.00	3.00	125.85	0.00
106.05	0.00	110.75	0.00	120.15	0.00	126.15	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
133.20	0.00	147.20	0.00	164.80	0.00	183.80	0.00
133.45	0.00	149.30	0.00	165.15	1.00	191.20	0.00
134.45	0.00	149.65	0.00	167.10	0.00	200.55	0.00
136.45	0.00	151.00	1.00	169.00	2.00	205.05	0.00
137.05	0.00	152.45	0.00	170.45	0.00	207.00	0.00
142.20	0.00	153.30	0.00	172.30	0.00	207.20	0.00
142.95	0.00	162.20	0.00	173.45	0.00	213.05	0.00
143.05	0.00	162.80	0.00	176.20	0.00	214.00	0.00
143.20	0.00	163.00	2.00	177.05	0.00	219.00	2.00
146.20	0.00	163.85	0.00	181.00	0.00	219.80	0.00
147.00	1.00	164.00	0.00	181.25	0.00	237.30	0.00

#3: 5-METHYL-3-HEXEN-2-ONE
Modified: scaled
Entry Number 3 from C:\DATABASE\hjf.l
CAS 005166-53-0
Melting Point -300
Boiling Point -300
Retention Index 39.42
Mol Formula C7H12O
Mol Weight 112.088

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	184.00	41.05	8214.00	56.05	91.00	67.05	682.00
26.90	1368.00	42.00	656.00	57.00	55.00	68.05	247.00

29.00	370.00	43.00	9999.00	58.00	209.00	69.05	4138.00
30.00	9.00	46.95	6.00	59.00	133.00	70.05	626.00
31.05	30.00	48.90	10.00	60.00	6.00	71.05	336.00
32.90	4.00	49.95	213.00	60.90	20.00	72.05	17.00
35.90	2.00	50.90	338.00	62.00	38.00	73.05	4.00
36.90	60.00	52.00	151.00	63.00	55.00	74.00	12.00
37.90	157.00	53.05	885.00	64.00	9.00	74.90	4.00
38.90	1540.00	54.00	289.00	65.05	128.00	77.05	226.00
40.00	253.00	55.05	1312.00	66.00	46.00	78.05	27.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
79.05	825.00	92.05	8.00	107.05	2.00	122.15	0.00
80.05	56.00	93.05	64.00	108.05	1.00	123.05	0.00
81.00	153.00	94.05	51.00	109.10	10.00	124.55	0.00
82.05	104.00	95.05	88.00	110.05	21.00	124.80	0.00
83.05	101.00	97.05	5399.00	111.10	141.00	125.05	0.00
83.95	7.00	98.05	339.00	112.15	4233.00	125.40	0.00
85.00	11.00	99.00	20.00	113.15	456.00	126.30	0.00
87.05	0.00	100.95	0.00	114.10	27.00	127.55	0.00
88.90	1.00	104.80	0.00	115.10	1.00	127.80	0.00
89.15	0.00	105.05	0.00	116.30	0.00	135.20	0.00
91.05	51.00	105.90	0.00	121.10	0.00	145.95	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
151.05	0.00						
153.20	1.00						
157.80	0.00						
175.95	0.00						
220.05	0.00						
229.55	0.00						

#4: 2-METHYLBENZALDEHYDE
Modified: scaled

Entry Number 4 from C:\DATABASE\hjf.l
CAS 000529-20-4
Melting Point -300
Boiling Point -300
Retention Index 53.56
Mol Formula C8H8O
Mol Weight 120.057
Miscellaneous Information
Aldrich: o-tolualdehyde

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	50.00	38.90	1639.00	52.05	147.00	63.05	1103.00
26.90	196.00	40.00	148.00	53.00	83.00	64.05	284.00
28.90	129.00	41.00	258.00	54.00	5.00	65.05	2627.00
29.95	1.00	42.00	16.00	55.00	11.00	66.05	173.00

30.90	2.00	44.95	41.00	56.00	0.00	67.00	9.00
32.90	0.00	45.80	55.00	56.95	1.00	68.00	2.00
33.10	1.00	46.90	3.00	58.00	1.00	71.00	1.00
33.80	0.00	47.95	5.00	59.05	81.00	72.00	3.00
35.90	7.00	48.90	48.00	60.00	136.00	73.00	31.00
36.90	121.00	49.90	482.00	60.95	163.00	74.00	149.00
37.90	269.00	51.00	749.00	62.00	432.00	75.05	107.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
76.05	65.00	87.00	72.00	97.05	4.00	107.90	0.00
77.05	143.00	88.00	18.00	98.05	12.00	108.55	0.00
78.05	26.00	89.05	838.00	99.00	3.00	109.10	0.00
79.05	6.00	90.05	414.00	101.00	5.00	111.55	0.00
80.10	1.00	91.05	9999.00	102.05	16.00	113.05	0.00
81.05	1.00	92.05	1040.00	103.00	10.00	115.05	1.00
81.80	0.00	93.05	45.00	104.05	2.00	116.10	2.00
81.90	0.00	94.05	2.00	105.05	22.00	117.10	3.00
83.95	5.00	94.80	0.00	106.00	2.00	119.05	8189.00
85.05	58.00	95.30	0.00	106.90	0.00	120.05	9115.00
86.00	94.00	96.00	0.00	107.10	0.00	121.05	768.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.05	46.00	131.80	0.00	153.15	1.00	195.20	0.00
123.10	2.00	136.20	0.00	154.15	0.00	195.95	0.00
124.10	0.00	138.05	0.00	155.00	0.00	196.20	1.00
125.90	0.00	139.10	1.00	167.10	0.00	197.20	0.00
126.10	0.00	140.05	0.00	168.15	1.00	211.20	3.00
127.05	0.00	141.10	1.00	170.70	0.00	212.25	0.00
127.15	0.00	142.15	1.00	176.10	0.00	213.70	0.00
127.30	0.00	143.20	0.00	182.10	0.00	220.30	0.00
128.10	2.00	148.05	0.00	183.15	4.00		
129.05	1.00	151.00	0.00	184.20	1.00		
130.05	0.00	152.15	1.00	193.15	1.00		

#5: 3-METHYLBENZALDEHYDE
Modified: scaled
Entry Number 5 from C:\DATABASE\hjf.l
CAS 000520-23-5
Melting Point -300
Boiling Point -300
Retention Index 54.228
Mol Formula C8H8O
Mol Weight 120.057
Miscellaneous Information
Aldrich: m-tolualdehyde

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	47.00	38.95	1605.00	54.00	4.00	67.05	5.00
26.95	187.00	39.95	142.00	55.00	4.00	69.80	0.00

28.90	142.00	41.00	276.00	56.20	1.00	70.40	0.00
29.95	1.00	42.05	13.00	59.00	73.00	71.95	2.00
32.95	0.00	44.90	16.00	60.00	41.00	72.95	31.00
33.30	0.00	47.95	5.00	60.90	160.00	74.05	148.00
34.40	0.00	48.90	43.00	62.00	420.00	75.05	107.00
35.05	0.00	49.90	483.00	63.05	1093.00	76.00	64.00
35.90	7.00	50.95	749.00	64.05	274.00	77.05	104.00
36.90	116.00	52.05	146.00	65.05	2612.00	78.05	19.00
37.90	259.00	53.00	89.00	66.00	169.00	79.00	4.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
80.05	0.00	93.05	42.00	106.90	0.00	123.10	2.00
80.65	0.00	94.05	2.00	107.10	0.00	123.90	0.00
83.95	6.00	97.05	2.00	109.90	0.00	124.30	0.00
85.00	63.00	98.05	8.00	112.95	0.00	126.90	0.00
86.00	106.00	99.05	2.00	115.05	1.00	127.10	0.00
87.05	75.00	101.05	3.00	116.05	2.00	128.15	1.00
88.00	15.00	102.05	10.00	117.15	6.00	129.05	1.00
89.05	813.00	103.05	9.00	119.05	8802.00	129.80	0.00
90.05	348.00	104.05	2.00	120.05	8937.00	130.15	0.00
91.05	9999.00	105.05	16.00	121.05	821.00	132.05	0.00
92.05	993.00	106.10	1.00	122.05	50.00	133.20	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
134.05	0.00	148.20	0.00	165.20	0.00	207.30	0.00
135.70	0.00	150.05	0.00	167.15	1.00	211.20	2.00
136.20	0.00	151.10	0.00	168.10	1.00	212.20	0.00
136.45	0.00	152.10	1.00	176.10	0.00	213.05	0.00
138.00	0.00	153.15	1.00	181.10	0.00	214.05	0.00
139.05	1.00	154.10	0.00	183.20	16.00	220.80	0.00
139.95	0.00	155.15	1.00	184.20	3.00	221.05	0.00
141.10	1.00	156.20	0.00	193.15	1.00		
142.15	1.00	157.20	0.00	196.20	1.00		
143.15	0.00	163.30	0.00	197.20	0.00		
144.05	0.00	163.80	0.00	207.05	0.00		

#6: 5-METHYL-2-FURANCARBOXALDEHYDE
Modified: scaled
Entry Number 6 from C:\DATABASE\hjf.l
CAS 000620-02-0
Melting Point -300
Boiling Point -300
Retention Index 47.798
Mol Formula C6H6O2
Mol Weight 110.04
Miscellaneous Information
Aldrich: 5-methylfurfural

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.

25.90	300.00	38.90	874.00	54.00	367.00	64.95	22.00
26.90	1620.00	39.90	52.00	54.90	78.00	65.90	28.00
27.90	102.00	40.90	109.00	55.90	12.00	66.90	47.00
28.90	445.00	41.90	147.00	57.00	0.00	67.95	13.00
29.90	13.00	42.95	825.00	57.90	11.00	68.90	36.00
30.90	12.00	47.90	17.00	58.90	1.00	69.90	8.00
32.65	0.00	48.90	135.00	59.90	11.00	70.95	4.00
33.60	0.00	49.90	759.00	60.90	31.00	71.95	1.00
35.90	29.00	50.90	1075.00	61.90	30.00	72.90	3.00
36.90	227.00	52.00	532.00	62.90	38.00	73.90	4.00
37.90	376.00	52.95	4187.00	64.00	17.00	74.80	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
74.90	0.00	87.15	0.00	97.90	0.00	109.05	8313.00
75.30	0.00	88.85	0.00	98.40	0.00	110.05	9999.00
76.00	1.00	89.90	0.00	98.65	0.00	111.05	775.00
76.90	10.00	90.10	0.00	99.10	0.00	112.05	64.00
78.05	2.00	90.95	1.00	101.00	0.00	113.00	4.00
79.00	182.00	92.00	1.00	101.40	0.00	114.90	0.00
80.05	140.00	92.90	4.00	101.65	0.00	115.15	0.00
81.05	1111.00	94.05	5.00	102.10	0.00	116.05	0.00
82.00	83.00	95.00	79.00	103.95	0.00	116.90	0.00
83.00	6.00	96.05	4.00	105.05	0.00	117.15	0.00
85.10	1.00	97.05	1.00	106.05	1.00	118.05	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
118.30	0.00	135.05	0.00	162.30	0.00	198.55	0.00
120.30	0.00	135.20	0.00	162.55	0.00	201.55	0.00
121.05	0.00	135.45	0.00	163.95	0.00		
122.95	0.00	136.45	0.00	164.20	0.00		
123.65	0.00	137.05	0.00	166.05	0.00		
123.95	0.00	142.95	0.00	168.20	0.00		
124.55	0.00	146.95	0.00	168.45	0.00		
124.80	0.00	147.20	0.00	169.20	0.00		
132.95	0.00	147.95	0.00	178.80	0.00		
133.30	0.00	159.05	0.00	180.80	0.00		
134.95	0.00	162.00	0.00	193.80	0.00		

#7: 3-METHYL-2(5H)-FURANONE
Modified: scaled
Entry Number 7 from C:\DATABASE\hjf.l
CAS 022122-36-7
Melting Point -300
Boiling Point -300
Retention Index 53.359
Mol Formula C5H6O2
Mol Weight 98.037

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.

25.90	447.00	37.90	637.00	53.95	99.00	62.90	0.00
26.90	1021.00	38.90	3905.00	54.90	105.00	63.00	0.00
27.90	342.00	40.00	1520.00	56.00	7.00	63.90	1.00
28.90	583.00	40.95	9999.00	57.00	2.00	64.95	3.00
29.90	35.00	42.00	530.00	57.90	1.00	65.90	15.00
30.90	65.00	47.90	25.00	58.90	1.00	66.95	39.00
33.00	10.00	48.90	112.00	59.05	0.00	68.00	648.00
33.90	42.00	49.90	461.00	59.95	0.00	69.00	9488.00
34.85	1.00	50.90	382.00	60.95	2.00	70.00	588.00
35.90	54.00	51.95	202.00	61.95	1.00	71.05	35.00
36.90	385.00	52.90	727.00	62.70	0.00	71.95	3.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
72.65	0.00	81.95	2.00	96.05	9.00	106.05	1.00
73.00	1.00	82.95	6.00	97.05	160.00	108.15	0.00
73.55	0.00	85.10	2.00	98.05	8817.00	110.00	0.00
73.95	0.00	86.80	1.00	99.00	621.00	114.95	1.00
75.65	0.00	89.00	0.00	100.00	52.00	116.80	0.00
76.30	0.00	91.00	0.00	101.05	3.00	118.15	0.00
76.95	2.00	92.80	0.00	102.15	0.00	120.05	0.00
78.00	1.00	93.05	0.00	104.00	0.00	120.90	0.00
79.00	3.00	94.00	0.00	104.30	0.00	132.80	0.00
79.95	1.00	94.35	1.00	105.00	0.00	145.20	0.00
80.95	4.00	95.05	1.00	105.35	0.00	146.10	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
146.80	0.00	230.95	0.00				
150.00	0.00	243.05	0.00				
150.85	1.00						
151.80	0.00						
163.95	1.00						
167.95	0.00						
169.00	0.00						
176.00	0.00						
180.80	0.00						
213.95	0.00						
217.05	0.00						

#8: 5-ETHYL-2-FURALDEHYDE
Modified: scaled
Entry Number 8 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 54.689
Mol Formula C7H8O2
Mol Weight 124.052

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.

25.90	240.00	40.90	2333.00	55.95	12.00	66.05	389.00
26.90	1265.00	41.90	161.00	57.00	56.00	67.05	3252.00
28.90	921.00	46.90	11.00	57.95	6.00	68.00	201.00
29.90	18.00	48.00	6.00	58.60	0.00	68.90	25.00
30.90	62.00	48.90	55.00	59.00	0.00	70.00	3.00
31.90	19.00	49.90	456.00	59.95	11.00	70.95	3.00
35.90	20.00	50.90	895.00	60.90	74.00	72.05	1.00
36.90	261.00	51.95	547.00	61.90	143.00	72.95	5.00
37.90	606.00	52.95	2653.00	62.95	282.00	73.95	12.00
38.90	2453.00	53.95	134.00	64.00	80.00	74.95	4.00
39.95	387.00	54.90	230.00	65.05	1193.00	75.95	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
77.00	72.00	89.95	0.00	103.20	0.00	117.25	0.00
78.00	12.00	90.30	0.00	103.80	0.00	117.80	0.00
78.95	174.00	91.00	3.00	105.05	23.00	118.05	0.00
80.05	153.00	92.00	5.00	105.95	2.00	118.95	5.00
81.05	2100.00	93.05	42.00	109.05	8116.00	120.05	0.00
82.00	116.00	95.05	4114.00	110.05	553.00	121.05	131.00
82.95	8.00	96.05	279.00	111.05	45.00	122.00	46.00
84.90	1.00	97.05	22.00	112.05	2.00	123.05	1864.00
87.10	0.00	98.90	0.00	112.80	0.00	124.05	9999.00
88.90	0.00	101.10	0.00	115.00	1.00	125.05	885.00
89.15	0.00	102.95	0.00	116.25	0.00	126.05	70.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
127.05	5.00	147.20	0.00	219.95	0.00		
128.00	0.00	148.25	0.00				
128.90	0.00	151.20	0.00				
131.95	0.00	156.90	0.00				
132.95	0.00	158.05	0.00				
134.20	0.00	163.05	0.00				
136.10	0.00	175.95	0.00				
137.05	2.00	201.20	0.00				
138.15	0.00	203.05	0.00				
142.05	0.00	205.15	1.00				
145.05	0.00	214.00	0.00				

#9: 1-(4-METHYLPHENYL)-ETHANONE
Modified: scaled
Entry Number 9 from C:\DATABASE\hjf.l
CAS 000122-00-9
Melting Point -300
Boiling Point -300
Retention Index 63.429
Mol Formula C9H10O
Mol Weight 134.073
Miscellaneous Information

Aldrich: 4'-methylacetophenone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	22.00	45.40	158.00	57.55	6.00	70.40	0.00
26.90	134.00	47.95	0.00	59.05	52.00	70.80	0.00
28.90	5.00	48.90	9.00	60.90	66.00	71.95	1.00
35.95	1.00	49.90	267.00	61.90	219.00	72.95	13.00
36.90	37.00	50.90	446.00	62.95	615.00	73.90	86.00
37.90	114.00	51.90	111.00	64.00	170.00	74.95	66.00
38.90	876.00	52.90	79.00	65.00	1877.00	76.00	54.00
39.90	69.00	53.95	4.00	66.00	117.00	77.05	233.00
40.90	196.00	54.95	7.00	66.95	4.00	78.05	63.00
42.00	40.00	56.00	0.00	67.95	0.00	79.00	70.00
42.90	764.00	57.05	2.00	70.15	0.00	80.00	4.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
81.00	0.00	94.05	0.00	106.05	9.00	117.05	24.00
82.15	0.00	95.70	0.00	106.90	0.00	119.05	9999.00
84.90	28.00	96.05	0.00	107.10	1.00	120.05	937.00
85.95	50.00	97.00	2.00	108.00	0.00	121.05	54.00
87.00	45.00	98.05	6.00	109.05	1.00	122.00	3.00
88.00	11.00	99.00	1.00	110.00	1.00	123.00	0.00
89.05	651.00	101.00	4.00	111.00	0.00	124.80	0.00
90.05	312.00	102.00	20.00	113.05	2.00	125.00	0.00
91.05	6980.00	103.05	73.00	113.95	1.00	125.85	0.00
92.05	585.00	104.05	28.00	115.05	31.00	128.05	0.00
93.05	20.00	105.05	96.00	116.00	5.00	129.10	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
129.90	0.00	143.05	0.00	155.05	0.00	170.95	0.00
131.00	5.00	143.20	0.00	155.20	0.00	171.95	0.00
132.05	7.00	146.15	0.00	156.45	0.00	173.80	0.00
134.05	3730.00	146.80	0.00	156.80	0.00	176.05	0.00
135.05	377.00	147.20	0.00	157.20	0.00	178.80	0.00
136.05	23.00	151.90	0.00	161.30	0.00	181.00	0.00
137.10	1.00	152.15	0.00	162.95	0.00	181.20	0.00
138.80	0.00	152.45	0.00	164.70	0.00	182.30	0.00
141.05	0.00	153.05	1.00	165.00	0.00	183.05	0.00
142.10	0.00	154.05	0.00	165.30	0.00	197.15	0.00
142.95	0.00	154.95	0.00	166.10	0.00	214.00	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
214.30	0.00						
223.70	0.00						
225.10	1.00						
226.05	0.00						

#10: 2,5-FURANDIONE
Modified: scaled

Entry Number 10 from C:\DATABASE\hjf.l
CAS 000108-31-6
Melting Point -300
Boiling Point -300
Retention Index 44.479
Mol Formula C4H2O3
Mol Weight 98
Miscellaneous Information
Aldrich: maleic anhydride

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	9972.00	37.90	20.00	55.00	323.00	67.00	0.00
26.90	396.00	38.95	1.00	55.95	30.00	68.05	8.00
27.90	463.00	39.90	92.00	56.75	1.00	68.90	26.00
28.90	298.00	40.90	516.00	57.15	1.00	69.90	9.00
29.90	3.00	41.90	93.00	58.15	1.00	70.95	1.00
31.00	1.00	44.90	52.00	59.05	1.00	72.30	1.00
31.90	47.00	47.95	1.00	60.40	1.00	73.00	0.00
32.95	1.00	50.90	1.00	61.60	1.00	73.30	1.00
33.60	2.00	51.90	265.00	61.90	1.00	74.05	1.00
35.90	139.00	52.90	1193.00	63.85	1.00	74.30	0.00
36.90	169.00	53.90	9999.00	65.85	1.00	74.90	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
76.30	0.00	94.10	1.00	105.10	1.00	139.20	0.00
79.90	2.00	95.05	5.00	107.05	0.00	146.70	0.00
80.95	1.00	96.00	10.00	109.10	0.00	147.05	0.00
82.00	54.00	98.05	3359.00	114.00	0.00	150.00	1.00
83.00	3.00	99.00	161.00	117.10	1.00	150.95	0.00
84.95	0.00	100.05	25.00	117.65	0.00	157.05	0.00
86.85	0.00	101.05	1.00	119.00	0.00	165.55	1.00
89.15	0.00	102.05	1.00	121.30	0.00	181.00	1.00
91.00	1.00	102.65	0.00	122.05	1.00	207.20	0.00
92.05	2.00	102.90	0.00	126.05	1.00	219.95	1.00
93.90	0.00	103.15	0.00	133.80	1.00		

#11: DIHYDRO-5-METHYL-2(3H)-FURANONE
Modified: scaled
Entry Number 11 from C:\DATABASE\hjf.l
CAS 000108-29-2
Melting Point -300
Boiling Point -300
Retention Index 51.85
Mol Formula C5H8O2
Mol Weight 100.052
Miscellaneous Information
Aldrich: gamma-valerolactone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	702.00	37.90	132.00	51.95	39.00	62.05	1.00
26.90	1996.00	38.90	1028.00	53.00	168.00	63.00	1.00
27.90	4486.00	40.00	299.00	54.00	100.00	63.65	0.00
28.90	4137.00	41.05	3562.00	55.05	893.00	64.05	1.00
30.00	83.00	41.95	564.00	56.05	9999.00	65.15	0.00
30.90	64.00	42.95	3055.00	57.05	1754.00	67.00	2.00
33.00	1.00	44.90	437.00	58.05	66.00	67.95	2.00
34.00	2.00	47.90	4.00	59.00	8.00	70.00	2.00
34.90	1.00	48.90	20.00	59.95	3.00	71.05	187.00
35.90	10.00	49.90	125.00	61.00	0.00	72.05	12.00
36.90	79.00	50.90	97.00	61.70	0.00	73.00	3.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
73.80	0.00	83.00	33.00	97.00	1.00	108.80	0.00
74.30	0.00	85.05	5885.00	98.05	2.00	109.15	0.00
74.80	0.00	86.00	235.00	99.05	427.00	110.55	0.00
75.05	0.00	87.00	27.00	100.05	875.00	112.15	1.00
75.40	0.00	89.10	0.00	101.05	271.00	113.10	1.00
77.00	0.00	90.05	0.00	102.00	16.00	114.00	0.00
78.00	0.00	91.00	0.00	103.05	1.00	115.05	1.00
78.95	0.00	92.30	0.00	104.00	0.00	118.05	0.00
79.15	0.00	93.00	0.00	105.90	0.00	120.10	0.00
81.05	41.00	95.05	3.00	107.05	0.00	122.05	0.00
82.05	7.00	96.10	0.00	108.55	0.00	123.30	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
125.65	0.00	164.10	0.00	214.00	0.00		
127.55	0.00	169.00	0.00	219.95	0.00		
128.15	0.00	176.00	0.00				
132.05	0.00	179.45	0.00				
133.30	0.00	188.95	0.00				
138.05	0.00	189.20	0.00				
139.05	0.00	193.45	0.00				
141.05	0.00	194.05	0.00				
144.95	0.00	198.95	0.00				
150.20	0.00	206.95	0.00				
156.80	0.00	207.20	0.00				

#12: 2H-PYRAN-2-ONE
Modified: scaled
Entry Number 12 from C:\DATABASE\hjf.l
CAS 000504-31-4
Melting Point -300
Boiling Point -300
Retention Index 52.45
Mol Formula C5H4O2
Mol Weight 96.021

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	593.00	40.00	3161.00	58.20	1.00	69.00	445.00
27.05	163.00	40.90	322.00	58.95	0.00	70.00	48.00
28.90	1116.00	41.90	1508.00	59.90	7.00	71.05	1.00
29.95	10.00	47.90	71.00	61.00	6.00	72.00	0.00
30.90	1.00	48.90	301.00	61.95	1.00	75.95	1.00
33.05	23.00	49.90	665.00	63.10	0.00	77.00	10.00
33.90	181.00	50.90	303.00	63.95	8.00	78.00	2.00
35.90	204.00	51.95	55.00	65.00	30.00	79.00	6.00
36.90	1265.00	52.90	197.00	66.00	88.00	80.05	7.00
37.90	2255.00	53.95	38.00	67.05	415.00	81.05	0.00
38.90	8549.00	54.95	10.00	68.05	8921.00	82.00	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
86.80	0.00	99.05	2.00	117.90	0.00	181.00	0.00
87.05	1.00	103.90	0.00	119.65	0.00	182.20	0.00
88.85	0.00	105.00	1.00	128.15	0.00	207.05	0.00
91.00	0.00	106.05	0.00	128.90	0.00		
91.85	0.00	107.05	1.00	135.10	1.00		
92.15	0.00	107.80	0.00	141.45	0.00		
92.95	9.00	110.05	0.00	144.95	0.00		
95.00	1821.00	111.05	0.00	145.20	0.00		
96.05	9999.00	112.10	0.00	146.95	0.00		
97.05	581.00	113.05	1.00	148.55	0.00		
98.05	52.00	116.15	0.00	149.20	0.00		

#13: 1(3H)-ISOBENZOFURANONE
Modified: scaled

Entry Number 13 from C:\DATABASE\hjf.l
CAS 000087-41-2
Melting Point -300
Boiling Point -300
Retention Index 80.92
Mol Formula C8H6O2
Mol Weight 134.037
Miscellaneous Information
Aldrich: phthalide

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	44.00	39.95	30.00	59.95	20.00	76.05	1020.00
26.95	124.00	47.90	10.00	60.90	116.00	77.05	4388.00
28.90	94.00	48.90	90.00	62.00	209.00	78.05	394.00
29.90	5.00	49.90	1102.00	63.05	441.00	79.05	20.00
30.95	3.00	50.95	1367.00	64.05	88.00	80.05	0.00
33.35	0.00	52.00	283.00	65.05	8.00	81.40	0.00
33.95	0.00	52.90	77.00	66.00	192.00	85.05	36.00

35.95	16.00	53.95	2.00	72.00	7.00	86.00	39.00
36.90	181.00	55.00	3.00	73.05	86.00	87.05	31.00
37.90	306.00	58.30	0.00	74.05	403.00	88.00	2.00
38.90	317.00	58.95	0.00	75.05	343.00	89.05	251.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
90.05	72.00	105.05	9999.00	118.10	4.00	135.05	423.00
91.05	5.00	106.05	810.00	119.05	3.00	136.05	35.00
92.05	1.00	107.05	44.00	120.00	0.00	137.10	2.00
92.65	0.00	108.05	2.00	121.10	0.00	138.10	0.00
94.10	0.00	109.10	0.00	125.15	0.00	139.10	1.00
97.40	0.00	111.10	0.00	126.30	0.00	140.25	0.00
101.05	3.00	112.15	0.00	127.10	0.00	141.15	0.00
101.90	0.00	115.05	1.00	128.10	1.00	142.05	0.00
102.10	1.00	115.95	0.00	129.10	0.00	143.05	0.00
103.05	31.00	116.05	0.00	133.05	1214.00	144.05	0.00
104.05	198.00	117.05	0.00	134.05	4055.00	144.45	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
144.70	0.00	166.15	1.00	184.15	1.00		
147.00	0.00	167.20	1.00	193.05	3.00		
150.20	0.00	168.15	0.00	194.15	2.00		
151.10	0.00	169.05	2.00	209.10	3.00		
152.10	1.00	170.25	0.00	210.10	1.00		
153.05	1.00	174.30	0.00	211.10	2.00		
154.20	1.00	176.00	0.00	212.15	0.00		
155.20	3.00	180.10	0.00				
156.15	1.00	181.05	1.00				
164.05	0.00	182.10	1.00				
165.05	3.00	183.10	4.00				

#14: BENZALDEHYDE
Modified: scaled
Entry Number 14 from C:\DATABASE\hjf.l
CAS 000100-52-7
Melting Point -300
Boiling Point -300
Retention Index 45.609
Mol Formula C7H6O
Mol Weight 106.042

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	100.00	40.95	1.00	58.00	1.00	70.80	0.00
26.90	315.00	47.90	20.00	59.90	26.00	72.00	14.00
28.90	215.00	48.90	189.00	60.95	99.00	73.00	161.00
29.90	2.00	49.90	1898.00	61.95	136.00	74.05	639.00
30.95	1.00	50.95	3513.00	63.00	204.00	75.05	313.00
33.90	0.00	52.00	902.00	64.00	25.00	76.05	444.00
35.90	28.00	52.90	138.00	65.00	3.00	77.05	9137.00

36.90	240.00	53.80	2.00	66.05	4.00	78.05	1387.00
37.90	318.00	54.05	1.00	66.95	1.00	79.05	77.00
38.90	541.00	54.95	5.00	68.00	1.00	80.05	3.00
39.90	21.00	55.85	1.00	70.15	0.00	80.90	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
81.30	0.00	91.05	1.00	109.05	2.00	141.20	0.00
81.80	0.00	93.40	0.00	110.05	0.00	146.05	0.00
83.05	1.00	94.15	0.00	115.05	2.00	150.00	0.00
83.90	7.00	95.80	0.00	117.05	0.00	151.05	0.00
85.00	28.00	101.05	3.00	117.90	0.00	153.10	3.00
86.00	26.00	101.95	1.00	120.05	1.00	154.15	2.00
87.05	14.00	103.05	4.00	127.05	1.00	155.15	19.00
87.95	2.00	105.05	9499.00	128.10	1.00	156.15	3.00
89.05	38.00	106.05	9999.00	129.10	1.00	157.20	0.00
90.05	8.00	107.05	849.00	139.05	0.00	164.05	0.00
90.90	0.00	108.05	49.00	140.95	0.00	165.10	2.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
181.20	0.00						
183.20	0.00						

#15: 4-METHYLBENZALDEHYDE
Modified: scaled
Entry Number 15 from C:\DATABASE\hjf.l
CAS 000104-87-0
Melting Point -300
Boiling Point -300
Retention Index 55.409
Mol Formula C8H8O
Mol Weight 120.057
Miscellaneous Information
Aldrich: p-tolualdehyde

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	41.00	36.90	108.00	50.90	703.00	59.80	14.00
26.95	165.00	37.90	243.00	52.00	131.00	60.90	154.00
28.90	123.00	38.90	1467.00	52.95	82.00	62.00	389.00
29.90	2.00	40.00	130.00	53.95	4.00	63.05	1017.00
30.95	4.00	41.00	254.00	54.95	4.00	64.00	263.00
32.85	0.00	42.05	14.00	56.05	1.00	65.05	2408.00
33.60	0.00	44.90	50.00	56.15	1.00	66.05	154.00
33.95	1.00	45.65	23.00	56.80	1.00	67.05	6.00
34.30	1.00	47.90	4.00	57.40	0.00	67.95	2.00
34.65	0.00	48.90	45.00	57.80	1.00	69.80	0.00
35.95	7.00	49.90	473.00	59.00	151.00	70.80	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
72.05	3.00	81.65	0.00	93.00	39.00	105.05	26.00
72.95	31.00	82.40	0.00	94.05	2.00	106.05	2.00

74.05	144.00	83.90	10.00	96.10	1.00	107.10	1.00
75.00	95.00	85.00	55.00	96.40	0.00	114.90	0.00
76.05	60.00	86.00	102.00	97.05	3.00	115.15	1.00
77.05	99.00	87.00	73.00	98.05	9.00	116.10	2.00
78.00	16.00	88.00	22.00	99.00	2.00	117.15	4.00
79.00	4.00	89.05	822.00	101.05	2.00	119.05	9999.00
79.80	1.00	90.05	362.00	102.05	10.00	120.05	9003.00
80.05	0.00	91.05	9482.00	103.05	10.00	121.05	798.00
81.05	1.00	92.05	913.00	104.05	4.00	122.05	50.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
123.05	3.00	164.05	0.00				
127.05	1.00	168.15	1.00				
128.10	1.00	169.00	0.00				
129.10	1.00	181.05	1.00				
130.15	0.00	183.20	8.00				
139.05	1.00	184.15	1.00				
142.10	1.00	193.10	1.00				
147.05	0.00	196.10	1.00				
152.05	1.00	211.15	1.00				
152.95	0.00						
153.20	1.00						

#16:2,5-DIMETHYLPHENOL
Modified: scaled
Entry Number 16 from C:\DATABASE\hjf.l
CAS 000105-67-9
Melting Point -300
Boiling Point -300
Retention Index 65.109
Mol Formula C8H10O
Mol Weight 122.072

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	64.00	37.85	160.00	49.90	320.00	60.05	474.00
26.95	481.00	38.90	953.00	50.90	842.00	60.95	187.00
28.90	69.00	39.95	149.00	51.95	334.00	62.00	149.00
29.90	2.00	41.00	352.00	53.00	592.00	63.00	355.00
31.00	16.00	42.00	35.00	53.90	61.00	64.05	94.00
32.85	3.00	43.05	264.00	55.05	223.00	65.00	684.00
33.70	1.00	44.90	91.00	56.05	9.00	66.00	163.00
34.90	0.00	45.90	98.00	57.05	2.00	67.00	115.00
35.90	1.00	46.90	19.00	57.80	1.00	68.00	21.00
36.15	2.00	47.90	3.00	58.05	1.00	68.95	5.00
36.90	49.00	48.90	23.00	59.05	117.00	70.00	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
72.05	1.00	83.00	5.00	95.05	47.00	108.05	786.00
72.95	16.00	85.05	13.00	96.05	7.00	109.05	46.00

73.95	82.00	85.95	18.00	97.05	3.00	110.10	2.00
75.05	68.00	87.00	22.00	98.05	9.00	115.05	0.00
76.00	73.00	88.00	4.00	99.05	3.00	116.15	0.00
77.05	2489.00	89.05	97.00	101.05	17.00	116.90	0.00
78.05	791.00	90.10	32.00	102.05	92.00	117.15	1.00
79.05	1459.00	91.05	1702.00	103.05	566.00	118.10	7.00
80.05	141.00	92.05	216.00	104.05	371.00	119.05	89.00
81.05	75.00	93.05	392.00	105.05	281.00	120.10	96.00
82.05	33.00	94.05	301.00	107.05	9951.00	121.05	4981.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.05	9999.00	158.20	0.00				
123.05	895.00	165.05	0.00				
124.10	55.00	166.00	1.00				
125.10	3.00	166.20	0.00				
129.30	0.00	169.05	0.00				
132.00	1.00	176.05	0.00				
134.20	0.00	181.05	0.00				
134.95	0.00						
135.20	0.00						
146.20	0.00						
148.45	0.00						

#17: CITRIC ACID
Modified: scaled
Entry Number 17 from C:\DATABASE\hjf.l
CAS 000077-92-9
Melting Point -300
Boiling Point -300
Retention Index 51.56
Mol Formula C6H8O7
Mol Weight 192.026

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.85	308.00	37.90	2358.00	48.90	66.00	65.00	13.00
26.95	186.00	38.90	9999.00	49.90	45.00	66.00	94.00
27.90	360.00	39.90	6688.00	50.95	8.00	67.05	244.00
28.90	157.00	40.90	333.00	51.90	79.00	67.95	8253.00
29.95	2.00	41.95	101.00	52.90	566.00	68.95	372.00
33.00	85.00	43.00	45.00	53.95	33.00	69.95	23.00
33.30	13.00	43.90	255.00	54.95	61.00	70.90	1.00
33.85	122.00	44.90	143.00	56.00	14.00	73.80	1.00
34.65	1.00	45.95	3.00	59.95	2.00	76.05	2.00
35.90	280.00	46.65	1.00	62.05	1.00	76.30	1.00
36.90	1503.00	47.95	45.00	63.95	9.00	77.05	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
78.90	1.00	87.80	1.00				
79.80	1.00	88.05	1.00				

79.90	1.00	94.90	1.00
80.05	1.00	96.00	17.00
80.85	2.00	99.90	0.00
81.05	1.00	112.05	352.00
82.05	1.00	113.00	59.00
82.95	8.00	113.95	3.00
83.95	4.00	132.00	2.00
85.05	1.00	150.05	1.00
85.90	1.00		

#18: 2,2-DIMETHYL-3(2H)-FURANONE
Modified: scaled
Entry Number 18 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 34.82
Mol Formula C6H8O2
Mol Weight 112.052

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	1048.00	37.90	263.00	51.95	27.00	63.95	4.00
26.90	661.00	38.90	1926.00	53.00	295.00	64.95	27.00
28.90	515.00	39.90	345.00	53.90	7067.00	66.05	19.00
29.95	10.00	40.95	1697.00	55.00	982.00	67.05	30.00
30.90	241.00	42.00	1307.00	56.05	84.00	68.05	21.00
33.00	1.00	42.90	8122.00	58.05	2894.00	68.90	663.00
33.35	1.00	46.95	0.00	59.05	5133.00	70.05	151.00
33.95	2.00	47.90	6.00	60.05	177.00	70.90	2640.00
35.05	1.00	48.90	25.00	60.95	24.00	72.05	97.00
35.95	12.00	49.95	80.00	61.95	14.00	73.05	27.00
36.90	128.00	50.90	68.00	62.95	11.00	73.95	4.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
77.00	0.00	95.05	23.00	115.05	5.00		
78.10	2.00	96.05	1.00	123.05	3.00		
79.00	0.00	97.05	320.00				
80.10	1.00	98.05	19.00				
80.95	9.00	99.05	2.00				
82.05	19.00	108.15	0.00				
83.05	129.00	109.00	4.00				
84.00	42.00	111.05	501.00				
85.00	7.00	112.05	9999.00				
86.05	0.00	113.05	760.00				
94.05	4.00	114.00	63.00				

#19: 2,5-HEXANEDIONE

Modified: scaled

Entry Number 19 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 46.609
Mol Formula C6H10O2
Mol Weight 114.067
Miscellaneous Information
Aldrich: acetonylacetone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.85	89.00	37.90	33.00	50.95	32.00	62.00	3.00
26.90	362.00	38.90	163.00	52.00	12.00	62.95	2.00
27.90	120.00	39.95	21.00	53.00	121.00	65.00	5.00
28.90	136.00	41.00	158.00	54.05	48.00	66.05	3.00
29.90	3.00	42.05	356.00	55.00	135.00	67.05	11.00
30.90	24.00	42.90	9999.00	56.05	25.00	68.00	3.00
32.95	0.00	44.90	19.00	57.05	652.00	68.90	4.00
33.95	1.00	46.95	0.00	58.05	33.00	71.05	1426.00
35.10	1.00	47.90	1.00	59.00	4.00	72.05	242.00
35.90	1.00	48.90	7.00	60.05	1.00	73.05	19.00
36.90	17.00	49.90	33.00	60.90	6.00	74.00	3.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
75.10	1.00	94.05	4.00	115.05	95.00		
77.05	3.00	95.05	22.00	116.05	8.00		
78.00	1.00	96.05	30.00	117.10	1.00		
79.00	2.00	97.05	19.00	169.00	0.00		
79.95	1.00	99.05	2992.00				
81.00	71.00	100.00	161.00				
82.05	6.00	101.05	15.00				
83.05	1.00	102.10	1.00				
84.00	0.00	111.05	0.00				
85.00	2.00	112.00	4.00				
86.00	3.00	114.00	688.00				

#20: 2,5-HEXANEDIONE
Modified: scaled

Entry Number 20 from C:\DATABASE\hjf.l
CAS 000616-02-4
Melting Point -300
Boiling Point -300
Retention Index 51.6
Mol Formula C5H4O3
Mol Weight 112.016

Miscellaneous Information
Aldrich: citraconic anhydride

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	315.00	40.90	343.00	54.95	61.00	73.90	1.00
27.00	208.00	41.90	107.00	56.05	13.00	77.00	0.00
28.90	167.00	44.90	81.00	57.10	3.00	77.95	0.00
29.95	4.00	46.95	1.00	60.00	3.00	80.05	3.00
32.95	101.00	47.90	46.00	64.00	7.00	81.05	1.00
33.90	107.00	48.85	66.00	64.95	12.00	83.00	7.00
35.90	285.00	49.90	49.00	65.95	90.00	84.00	8.00
36.90	1556.00	50.95	10.00	67.00	258.00	91.05	1.00
37.90	2363.00	51.90	82.00	68.05	8700.00	95.05	1.00
38.90	9999.00	52.90	576.00	68.95	370.00	95.15	1.00
40.00	6861.00	53.95	33.00	70.05	23.00	95.30	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
96.05	17.00						
99.05	2.00						
112.05	411.00						
113.05	69.00						
114.05	5.00						
132.00	0.00						
169.00	2.00						
219.95	1.00						

#21: 3-NITROTOLUENE
Modified: scaled

Entry Number 21 from C:\DATABASE\hjf.l
CAS 000099-08-1
Melting Point -300
Boiling Point -300
Retention Index 65.09
Mol Formula C7H7NO2
Mol Weight 137.048

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	37.00	39.90	115.00	53.95	12.00	72.00	1.00
27.00	144.00	41.05	384.00	58.40	1.00	73.00	23.00
29.90	307.00	42.00	13.00	59.95	12.00	74.05	123.00
33.30	0.00	45.90	10.00	60.90	122.00	75.05	105.00
33.80	1.00	46.90	0.00	62.00	380.00	76.05	69.00
34.65	0.00	47.95	5.00	63.05	1165.00	77.00	728.00
35.05	1.00	48.95	41.00	64.05	339.00	78.05	128.00
36.00	6.00	49.90	438.00	65.00	5321.00	79.00	834.00
36.90	91.00	51.00	671.00	66.05	297.00	80.05	62.00
37.90	228.00	52.05	182.00	67.05	10.00	81.05	6.00

38.90	1679.00	53.05	137.00	68.05	3.00	82.05	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
85.05	11.00	102.05	2.00	120.05	42.00	150.00	0.00
86.05	83.00	103.05	3.00	121.05	102.00	182.20	0.00
87.05	66.00	104.05	21.00	122.05	11.00	184.20	2.00
88.05	25.00	105.05	12.00	123.05	3.00		
89.05	1027.00	106.05	59.00	125.30	0.00		
90.05	445.00	107.05	1126.00	131.95	1.00		
91.05	9999.00	108.05	86.00	133.10	2.00		
92.05	784.00	109.05	6.00	135.05	14.00		
93.05	25.00	116.05	1.00	137.05	6813.00		
93.95	3.00	117.10	1.00	138.05	563.00		
95.05	2.00	118.10	3.00	139.05	47.00		

#22: DIHYDRO-2-METHYLENE-2,5-FURANDIONE
Modified: scaled

Entry Number 22 from C:\DATABASE\hjf.l
CAS 002170-03-8
Melting Point -300
Boiling Point -300
Retention Index 51.5
Mol Formula C5H4O3
Mol Weight 112.016
Miscellaneous Information
Aldrich: itaconic anhydride

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	305.00	36.90	1514.00	48.90	65.00	59.90	2.00
26.95	201.00	37.90	2322.00	49.90	47.00	60.80	1.00
27.90	463.00	38.90	9999.00	50.90	6.00	60.90	2.00
28.90	164.00	39.95	6751.00	51.85	87.00	61.80	1.00
29.95	1.00	40.95	330.00	52.90	565.00	63.90	3.00
30.90	4.00	41.95	102.00	53.95	41.00	64.05	6.00
33.05	97.00	43.90	116.00	54.95	60.00	64.90	15.00
33.60	15.00	44.90	137.00	56.00	12.00	65.30	1.00
33.95	117.00	45.90	4.00	57.00	3.00	65.95	100.00
34.60	1.00	47.05	6.00	58.10	4.00	67.00	251.00
35.90	280.00	47.95	46.00	58.90	2.00	68.00	8882.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
68.90	402.00	84.80	2.00	207.05	1.00		
69.95	27.00	87.05	3.00	219.00	1.00		
70.90	1.00	90.90	4.00	220.05	1.00		
75.00	1.00	92.05	2.00				
79.15	1.00	95.05	1.00				
80.05	1.00	96.00	21.00				
81.05	3.00	112.05	306.00				

81.95	1.00	113.05	49.00
83.00	8.00	113.95	6.00
83.30	2.00	114.95	2.00
83.90	5.00	119.00	3.00

#23: 2-METHYLBENZENE METHANOL
Modified: scaled

Entry Number 23 from C:\DATABASE\hjf.l
CAS 000089-95-2
Melting Point -300
Boiling Point -300
Retention Index 62.7
Mol Formula C8H10O
Mol Weight 122.072
Miscellaneous Information
Aldrich: 2-methylbenzyl alcohol

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	42.00	40.00	119.00	51.00	1180.00	60.80	93.00
27.00	376.00	41.05	275.00	52.00	371.00	61.95	229.00
28.90	156.00	42.00	25.00	53.00	269.00	63.00	645.00
29.95	10.00	44.90	1.00	53.95	19.00	64.05	151.00
30.95	116.00	45.90	24.00	55.00	51.00	65.05	1506.00
32.95	1.00	46.95	11.00	56.00	2.00	66.05	135.00
34.15	1.00	47.80	1.00	57.00	2.00	67.05	27.00
35.95	3.00	47.90	2.00	57.65	1.00	68.00	8.00
36.90	57.00	48.05	2.00	58.05	1.00	70.00	0.00
37.90	171.00	48.95	34.00	59.00	48.00	71.75	1.00
38.95	1141.00	49.95	396.00	60.05	402.00	71.90	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
72.05	1.00	83.10	2.00	94.05	129.00	106.10	106.00
73.00	20.00	84.00	7.00	95.00	10.00	107.05	2649.00
74.00	117.00	85.05	24.00	96.00	2.00	108.05	195.00
75.05	94.00	86.00	49.00	97.00	5.00	109.05	14.00
76.05	115.00	87.05	41.00	98.05	16.00	110.15	1.00
77.05	3283.00	88.00	12.00	99.05	5.00	112.05	1.00
78.05	1793.00	89.05	381.00	101.05	14.00	115.05	2.00
79.05	3771.00	90.05	111.00	102.05	152.00	116.00	3.00
80.05	244.00	91.05	3549.00	103.05	1351.00	117.10	3.00
81.00	21.00	92.05	350.00	104.05	9999.00	118.05	5.00
82.00	4.00	93.05	1599.00	105.05	1471.00	119.05	377.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
120.05	175.00						
121.05	397.00						
122.05	2362.00						
123.05	202.00						

124.05	14.00
125.15	0.00
128.10	2.00
154.15	1.00
169.00	2.00
181.00	0.00
207.20	1.00

#24: 4-ETHYL-1,2-BENZENEDIOL
Modified: scaled

Entry Number 24 from C:\DATABASE\hjf.l
CAS 002896-60-8
Melting Point -300
Boiling Point -300
Retention Index 85.7
Mol Formula C8H10O2
Mol Weight 138.068
Miscellaneous Information
Aldrich: 4-ethylresorcinol

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	44.00	41.00	482.00	54.95	484.00	67.05	930.00
26.90	309.00	41.90	93.00	56.05	11.00	68.05	187.00
28.90	121.00	42.95	455.00	57.05	25.00	68.90	580.00
29.95	2.00	45.90	2.00	58.05	3.00	69.95	17.00
30.95	2.00	47.40	74.00	59.05	28.00	73.05	6.00
33.95	0.00	48.90	19.00	60.05	5.00	74.00	31.00
36.00	2.00	49.90	156.00	61.55	154.00	75.05	34.00
36.90	35.00	51.05	365.00	63.00	195.00	76.05	23.00
37.90	115.00	52.05	134.00	64.05	60.00	77.05	517.00
38.90	649.00	53.05	422.00	65.05	608.00	78.05	72.00
40.00	133.00	54.05	142.00	66.05	230.00	79.05	227.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
80.05	42.00	93.05	56.00	108.05	25.00	124.05	812.00
81.05	210.00	94.05	138.00	109.05	93.00	125.05	70.00
82.05	44.00	95.05	693.00	110.05	57.00	126.10	2.00
84.05	0.00	96.05	48.00	111.05	11.00	129.10	0.00
86.05	6.00	101.05	12.00	116.05	0.00	133.10	0.00
87.05	8.00	102.05	6.00	117.05	1.00	134.05	16.00
88.10	3.00	103.05	19.00	118.05	12.00	135.05	33.00
89.05	63.00	104.05	2.00	119.05	73.00	136.05	61.00
90.05	29.00	105.05	29.00	120.05	66.00	137.10	273.00
91.05	359.00	106.05	6.00	121.05	121.00	138.05	4622.00
92.05	42.00	107.05	95.00	123.05	9999.00	139.05	427.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
140.10	36.00	179.10	0.00				

141.20	0.00	187.10	1.00
145.15	0.00	194.05	0.00
148.20	0.00	197.20	0.00
149.15	0.00		
150.05	0.00		
151.05	0.00		
160.15	1.00		
161.05	0.00		
163.10	0.00		
171.05	0.00		

#25: 1-(2,4-DIHYDROXYPHENYL)-ETHANONE
Modified: scaled

Entry Number 25 from C:\DATABASE\hjf.l
CAS 000089-84-9
Melting Point -300
Boiling Point -300
Retention Index 88.17
Mol Formula C8H8O3
Mol Weight 152.046
Miscellaneous Information
Aldrich: 2', 4'-dihydroxyacetophenone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	44.00	38.95	350.00	53.05	660.00	64.05	50.00
26.95	296.00	40.00	52.00	54.05	105.00	65.05	91.00
28.90	125.00	41.00	228.00	55.05	265.00	66.05	67.00
29.95	3.00	42.00	115.00	56.05	119.00	67.05	98.00
30.95	2.00	43.05	1079.00	57.05	334.00	68.90	721.00
34.00	3.00	47.05	17.00	58.05	17.00	70.05	56.00
34.90	1.00	47.90	20.00	58.95	0.00	71.05	229.00
35.10	1.00	48.95	31.00	60.00	7.00	72.05	13.00
35.95	4.00	49.95	164.00	61.00	50.00	73.05	6.00
36.90	55.00	51.00	336.00	62.05	258.00	74.05	24.00
37.90	125.00	52.05	226.00	63.00	202.00	75.05	16.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
76.05	18.00	87.05	3.00	98.10	7.00	109.05	583.00
77.05	161.00	88.05	1.00	99.10	73.00	110.05	74.00
78.05	58.00	89.05	3.00	100.05	4.00	111.10	22.00
79.05	85.00	90.05	8.00	101.05	0.00	112.15	6.00
80.05	108.00	91.05	17.00	102.10	0.00	113.10	52.00
81.05	1179.00	92.05	17.00	103.05	1.00	114.05	4.00
82.05	108.00	93.05	18.00	104.10	1.00	115.05	1.00
83.05	35.00	94.05	10.00	105.05	79.00	116.05	0.00
84.05	13.00	95.05	89.00	106.05	16.00	118.05	1.00
85.05	156.00	96.05	11.00	107.05	45.00	119.05	8.00

86.05	15.00	97.10	27.00	108.05	138.00	120.05	3.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.05	1.00	134.05	16.00	149.20	24.00	163.20	49.00
123.05	87.00	135.10	72.00	150.20	4.00	164.15	5.00
124.10	10.00	137.05	9999.00	152.05	4874.00	165.15	1.00
125.15	11.00	138.05	800.00	153.05	476.00	166.15	2.00
126.15	4.00	139.05	92.00	154.05	52.00	167.20	3.00
127.15	41.00	140.15	8.00	155.20	29.00	168.20	1.00
128.10	4.00	141.20	31.00	156.20	3.00	169.15	21.00
129.10	1.00	142.15	4.00	157.15	1.00	170.25	3.00
130.10	0.00	146.15	1.00	158.20	0.00	171.15	1.00
132.10	1.00	147.10	1.00	161.15	1.00	175.15	0.00
133.05	4.00	148.10	1.00	162.15	2.00	178.15	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
179.10	1.00	196.25	1.00	213.05	0.00		
180.15	1.00	197.25	8.00	214.20	0.00		
181.15	1.00	198.25	2.00	218.20	0.00		
182.20	2.00	199.20	0.00	221.20	0.00		
183.25	15.00	205.20	0.00	223.20	0.00		
184.10	0.00	207.05	0.00	224.25	5.00		
185.15	0.00	208.10	1.00	225.30	7.00		
189.15	1.00	209.10	0.00	226.25	1.00		
193.10	1.00	210.25	1.00	228.30	0.00		
194.15	1.00	211.20	5.00	234.25	1.00		
195.10	1.00	212.20	1.00				

#26: 2-ACETYL-5-METHYLFURAN
Modified: scaled

Entry Number 26 from C:\DATABASE\hjf.l
CAS 001193-79-9
Melting Point -300
Boiling Point -300
Retention Index 52.78
Mol Formula C7H8O2
Mol Weight 124.052

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	116.00	37.95	115.00	52.00	397.00	60.95	20.00
26.95	648.00	39.00	280.00	53.05	2048.00	61.95	33.00
28.90	20.00	40.00	25.00	54.05	238.00	63.05	33.00
30.95	7.00	40.90	82.00	54.95	42.00	63.95	10.00
32.80	1.00	41.95	113.00	56.00	7.00	65.00	45.00
33.05	1.00	43.05	1669.00	57.00	1.00	66.00	24.00
33.30	0.00	46.95	2.00	58.65	0.00	67.00	22.00
33.95	2.00	47.95	6.00	58.85	1.00	67.95	4.00
35.05	1.00	48.90	51.00	59.05	0.00	69.95	2.00

35.90	4.00	49.95	326.00	59.30	0.00	71.00	2.00
36.90	58.00	50.95	516.00	60.00	5.00	72.05	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
73.00	4.00	83.00	14.00	94.05	14.00	109.05	9999.00
73.95	5.00	83.95	1.00	95.05	80.00	110.05	677.00
74.95	2.00	84.95	2.00	96.05	7.00	111.05	65.00
75.90	0.00	85.75	1.00	96.90	1.00	112.05	5.00
76.10	1.00	86.05	1.00	97.10	1.00	114.00	0.00
77.00	21.00	87.80	0.00	103.05	0.00	119.05	0.00
78.05	9.00	89.40	0.00	104.40	0.00	120.05	0.00
79.00	78.00	91.05	2.00	105.00	4.00	122.30	0.00
80.05	73.00	91.95	3.00	105.75	1.00	123.05	5.00
81.05	705.00	92.05	1.00	106.10	2.00	124.05	4181.00
82.05	60.00	93.05	11.00	107.10	10.00	125.05	339.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
126.05	31.00						
127.10	2.00						
136.80	0.00						
143.20	0.00						
149.95	0.00						
164.05	0.00						
169.00	1.00						
191.20	0.00						

#27: 4-METHYL-2-NITROPHENOL
Modified: scaled

Entry Number 27 from C:\DATABASE\hjf.l
CAS 000119-33-5
Melting Point -300
Boiling Point -300
Retention Index 67.379
Mol Formula C7H7NO3
Mol Weight 153.042

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	123.00	35.90	15.00	48.90	86.00	59.00	2.00
26.95	616.00	36.90	118.00	49.95	857.00	60.00	13.00
28.90	111.00	37.95	245.00	51.00	2064.00	60.95	96.00
29.90	320.00	39.00	1348.00	52.00	1590.00	61.95	241.00
31.00	20.00	39.95	148.00	53.00	1970.00	63.00	679.00
32.95	10.00	41.00	348.00	54.00	161.00	64.00	209.00
33.80	3.00	41.90	47.00	54.90	776.00	65.05	1120.00
34.10	4.00	45.90	5.00	56.00	41.00	66.00	354.00
34.55	3.00	46.95	13.00	57.00	16.00	67.05	926.00
34.90	2.00	47.80	3.00	58.30	1.00	68.00	86.00
35.30	1.00	48.05	5.00	58.65	1.00	68.90	21.00

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
70.05	8.00	79.05	1010.00	90.05	36.00	101.90	1.00
70.85	3.00	80.05	138.00	91.05	69.00	102.15	1.00
71.05	1.00	81.00	111.00	92.05	197.00	103.05	6.00
71.30	1.00	82.05	27.00	93.00	45.00	104.05	4.00
71.95	4.00	83.05	8.00	94.05	89.00	105.05	1477.00
72.95	32.00	84.00	11.00	95.00	1048.00	106.05	520.00
74.00	145.00	85.00	17.00	96.05	76.00	107.05	1394.00
75.05	109.00	85.95	24.00	97.10	8.00	108.05	519.00
76.00	265.00	87.05	30.00	98.05	1.00	109.05	76.00
77.05	5432.00	88.05	15.00	99.00	2.00	110.05	9.00
78.05	2459.00	89.05	73.00	101.05	8.00	111.15	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
112.05	1.00	135.05	597.00	164.00	2.00		
118.05	5.00	136.05	611.00	176.05	1.00		
119.00	9.00	137.05	140.00				
120.05	182.00	138.15	15.00				
121.05	24.00	150.00	6.00				
122.05	28.00	151.05	35.00				
123.05	888.00	152.05	183.00				
124.05	75.00	153.05	9999.00				
125.05	8.00	154.05	822.00				
132.05	6.00	155.05	89.00				
133.10	8.00	156.10	7.00				

#28: 2-HYDROXY-5-METHOXYBENZALDEHYDE
Modified: scaled

Entry Number 28 from C:\DATABASE\hjf.l
CAS 000672-13-9
Melting Point -300
Boiling Point -300
Retention Index 72.319
Mol Formula C8H8O3
Mol Weight 152.046

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	209.00	35.90	14.00	48.90	44.00	60.00	20.00
27.00	517.00	36.95	107.00	49.90	304.00	60.95	135.00
28.90	361.00	37.95	233.00	51.00	531.00	61.95	274.00
29.90	14.00	38.95	654.00	52.05	786.00	63.00	672.00
31.00	22.00	39.90	50.00	52.90	2427.00	64.00	188.00
32.95	1.00	40.95	235.00	53.95	406.00	65.05	493.00
33.15	1.00	42.05	58.00	54.95	1064.00	66.00	145.00
34.10	4.00	46.90	28.00	56.00	45.00	67.05	112.00
34.30	2.00	47.70	4.00	57.00	14.00	68.00	27.00
34.75	1.00	47.90	5.00	58.10	2.00	68.90	219.00

35.10	3.00	48.00	2.00	58.95	13.00	70.00	14.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
71.00	12.00	80.05	276.00	91.05	98.00	104.05	11.00
71.80	1.00	81.00	1667.00	92.05	113.00	105.05	18.00
71.90	1.00	82.05	154.00	93.00	175.00	106.05	614.00
72.05	1.00	83.00	28.00	94.05	50.00	107.05	320.00
72.95	33.00	83.90	9.00	95.05	609.00	108.05	443.00
74.00	113.00	85.00	10.00	96.05	56.00	109.05	1891.00
75.05	128.00	86.05	7.00	97.00	14.00	110.05	134.00
76.00	91.00	88.15	3.00	98.10	3.00	111.05	15.00
77.05	98.00	88.40	1.00	99.15	1.00	111.95	2.00
78.00	24.00	89.05	4.00	101.05	5.00	116.90	1.00
79.05	284.00	90.05	17.00	103.05	4.00	119.05	30.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
120.00	18.00	137.05	6427.00	155.10	10.00		
121.05	63.00	138.05	515.00	164.20	1.00		
122.05	75.00	139.05	60.00	169.00	1.00		
123.05	490.00	140.05	2.00	181.00	1.00		
124.05	72.00	148.05	1.00	219.05	2.00		
125.05	13.00	149.10	12.00				
131.90	1.00	150.00	169.00				
132.05	1.00	151.05	1535.00				
133.20	1.00	152.05	9999.00				
134.05	141.00	153.05	898.00				
135.05	116.00	154.05	98.00				

#29: 3,4-DIMETHYLBENZOIC ACID
Modified: scaled

Entry Number 29 from C:\DATABASE\hjf.l
CAS 000619-04-5
Melting Point -300
Boiling Point -300
Retention Index 82.359
Mol Formula C9H10O2
Mol Weight 150.068

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	30.00	42.00	10.00	54.00	27.00	65.05	481.00
26.90	411.00	43.00	133.00	55.00	68.00	65.95	194.00
28.95	42.00	44.90	149.00	56.05	4.00	66.90	37.00
32.95	1.00	45.90	8.00	57.05	8.00	68.05	5.00
35.15	0.00	46.95	2.00	58.00	1.00	70.05	0.00
35.90	2.00	47.95	0.00	59.00	63.00	71.05	4.00
36.90	36.00	48.95	33.00	59.95	22.00	72.10	2.00
37.95	116.00	49.95	365.00	60.95	59.00	73.00	30.00
38.90	776.00	51.00	1113.00	62.00	189.00	74.05	351.00

39.95	74.00	52.00	262.00	63.00	536.00	75.00	140.00
41.00	144.00	53.00	387.00	64.00	121.00	76.05	141.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
77.05	2339.00	88.00	13.00	99.05	10.00	110.10	3.00
78.05	786.00	89.05	237.00	100.00	0.00	111.10	1.00
79.05	1670.00	90.05	92.00	101.05	37.00	112.05	0.00
80.05	114.00	91.05	3618.00	102.05	196.00	113.05	1.00
81.05	18.00	92.05	285.00	103.05	1339.00	115.05	3.00
82.05	4.00	93.05	54.00	104.05	735.00	116.10	7.00
83.05	2.00	94.05	11.00	105.05	9999.00	117.05	16.00
83.95	3.00	95.05	5.00	106.05	1268.00	118.05	15.00
85.05	18.00	96.10	1.00	107.05	356.00	119.05	43.00
86.00	39.00	97.05	8.00	108.05	26.00	120.05	11.00
87.05	44.00	98.05	31.00	109.05	3.00	121.05	201.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.05	35.00	133.05	2803.00	147.05	9.00	165.10	2.00
123.05	6.00	134.05	275.00	148.05	57.00	166.05	0.00
124.15	2.00	135.05	1050.00	149.05	454.00	167.05	3.00
125.10	1.00	136.05	97.00	150.05	8249.00	168.15	1.00
126.05	1.00	137.05	12.00	151.05	843.00	169.05	0.00
127.10	2.00	138.15	3.00	152.10	73.00	181.05	0.00
128.10	1.00	140.20	0.00	153.05	6.00	207.05	1.00
129.05	12.00	141.15	0.00	154.05	1.00	209.05	1.00
130.10	2.00	143.10	2.00	155.25	1.00	211.05	0.00
131.05	97.00	144.05	0.00	158.05	0.00	219.00	1.00
132.05	422.00	146.05	0.00	164.00	2.00	220.05	0.00

#30: 1-(PHENYL)-ETHANONE
Modified: scaled

Entry Number 30 from C:\DATABASE\hjf.l
CAS 000098-86-2
Melting Point -300
Boiling Point -300
Retention Index 54.53
Mol Formula C8H8O
Mol Weight 120.057
Miscellaneous Information
Aldrich: acetophenone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	27.00	39.90	18.00	53.95	2.00	65.95	11.00
26.90	143.00	41.00	25.00	55.00	1.00	66.90	0.00
28.90	6.00	41.95	71.00	55.90	1.00	67.05	1.00
31.00	0.00	42.95	1031.00	56.25	1.00	70.90	0.00
32.85	0.00	46.85	0.00	59.00	2.00	72.00	3.00
33.65	0.00	47.05	0.00	59.95	8.00	72.95	58.00

34.10	0.00	47.95	4.00	60.95	52.00	74.00	288.00
35.95	5.00	48.95	62.00	61.95	102.00	75.05	172.00
36.95	65.00	49.90	790.00	63.00	180.00	76.05	277.00
38.05	171.00	50.95	2140.00	64.00	34.00	77.05	7117.00
38.90	313.00	52.00	219.00	65.00	154.00	78.00	730.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
79.00	31.00	92.05	12.00	103.05	29.00	120.00	3343.00
80.05	1.00	93.00	1.00	105.05	9999.00	121.05	293.00
81.00	1.00	94.05	0.00	106.05	778.00	122.05	18.00
84.00	4.00	94.30	0.00	107.05	45.00	123.10	1.00
85.05	10.00	95.05	2.00	108.05	2.00	128.10	1.00
86.05	18.00	96.00	1.00	112.30	0.00	129.05	0.00
87.05	14.00	97.00	3.00	115.10	0.00	132.10	1.00
88.05	4.00	98.05	10.00	116.10	0.00	133.05	0.00
89.05	75.00	99.00	2.00	117.10	2.00	150.80	0.00
90.05	16.00	101.05	4.00	117.90	0.00	154.05	0.00
91.05	123.00	102.05	14.00	118.10	1.00	169.05	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
219.95	0.00						

#31: A-METHYLBENZENE ACETIC ACID
Modified: scaled

Entry Number 31 from C:\DATABASE\hjf.l
CAS 000492-37-5
Melting Point -300
Boiling Point -300
Retention Index 77.26
Mol Formula C9H10O2
Mol Weight 150.068
Miscellaneous Information
Aldrich: 2-phenylpropionic acid

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	23.00	36.90	18.00	48.95	16.00	59.95	7.00
26.90	278.00	37.95	52.00	49.90	234.00	60.90	23.00
27.90	5.00	38.90	295.00	51.00	730.00	62.00	68.00
28.90	19.00	39.95	25.00	52.00	158.00	63.00	198.00
29.95	1.00	41.00	27.00	52.90	111.00	64.05	41.00
32.80	1.00	41.95	3.00	54.05	8.00	65.00	125.00
34.30	0.00	43.00	71.00	55.00	21.00	66.00	26.00
34.55	0.00	44.90	81.00	56.00	3.00	67.00	4.00
34.95	0.00	45.95	3.00	57.05	2.00	70.05	0.00
35.30	0.00	46.95	1.00	58.10	2.00	71.05	2.00
35.95	2.00	47.95	1.00	59.00	0.00	71.95	2.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.

72.95	16.00	83.95	1.00	95.05	4.00	107.05	103.00
74.00	88.00	85.05	4.00	96.05	1.00	108.05	5.00
75.00	71.00	86.00	10.00	97.05	4.00	109.05	1.00
76.05	84.00	87.00	14.00	98.05	10.00	109.90	0.00
77.05	1603.00	88.00	3.00	99.05	3.00	110.15	0.00
78.05	520.00	89.05	109.00	101.05	15.00	111.10	1.00
79.05	1690.00	90.05	39.00	102.05	107.00	111.30	0.00
80.05	110.00	91.05	722.00	103.05	1094.00	112.05	0.00
81.05	5.00	92.05	55.00	104.05	383.00	115.05	2.00
82.00	1.00	93.05	6.00	105.05	9999.00	116.05	2.00
83.05	1.00	94.05	17.00	106.05	1138.00	117.10	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
118.05	4.00	131.05	3.00	151.05	272.00		
119.05	1.00	132.05	29.00	152.10	24.00		
120.10	2.00	133.05	6.00	153.10	2.00		
121.05	6.00	134.05	4.00	164.05	0.00		
122.05	3.00	135.05	17.00	167.10	1.00		
123.10	1.00	136.10	3.00	169.00	0.00		
124.15	0.00	137.05	2.00	181.05	1.00		
125.15	0.00	145.20	0.00				
126.05	0.00	147.10	3.00				
129.05	1.00	148.05	5.00				
129.90	0.00	150.05	2695.00				

#32: 1-ETHYL-4-NITROBENZENE
Modified: scaled

Entry Number 32 from C:\DATABASE\hjf.l
CAS 000100-12-9
Melting Point -300
Boiling Point -300
Retention Index 73.209
Mol Formula C8H9NO2
Mol Weight 151.062
Miscellaneous Information
Aldrich: 4-ethylnitrobenzene

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	66.00	41.00	199.00	55.00	90.00	65.05	779.00
26.95	1005.00	42.00	16.00	55.95	5.00	66.00	121.00
29.00	188.00	45.90	23.00	56.80	1.00	67.00	24.00
29.90	1063.00	47.10	3.00	57.10	3.00	68.05	7.00
33.05	1.00	48.05	1.00	58.30	1.00	69.95	0.00
34.00	1.00	48.95	53.00	58.60	4.00	70.90	2.00
36.00	3.00	49.90	973.00	59.95	8.00	72.00	4.00
36.90	73.00	50.95	1975.00	61.00	101.00	73.05	47.00
37.90	215.00	52.05	480.00	61.95	356.00	74.05	392.00

38.90	1376.00	53.00	573.00	63.00	1226.00	74.95	337.00
40.00	154.00	54.00	39.00	64.00	359.00	76.05	425.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
77.05	6673.00	88.05	33.00	98.05	40.00	109.10	3.00
78.05	2705.00	89.05	1434.00	99.05	14.00	116.10	7.00
79.05	4970.00	90.05	680.00	100.05	1.00	117.05	8.00
80.05	325.00	91.05	1066.00	101.05	54.00	118.05	25.00
81.05	14.00	92.05	176.00	102.05	389.00	119.05	32.00
81.95	2.00	93.05	942.00	103.05	3248.00	120.00	43.00
83.05	2.00	94.00	74.00	104.05	1557.00	121.05	982.00
84.00	6.00	95.05	7.00	105.05	6371.00	122.05	84.00
85.05	23.00	95.90	1.00	106.05	2130.00	123.05	21.00
86.05	65.00	96.10	1.00	107.05	198.00	124.10	7.00
87.00	80.00	97.05	8.00	108.05	12.00	124.90	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
128.30	1.00	147.20	1.00				
129.90	1.00	148.15	1.00				
132.05	4.00	149.10	9.00				
133.15	15.00	151.05	9999.00				
134.05	1221.00	152.10	917.00				
135.05	352.00	153.05	76.00				
136.05	2260.00	154.15	6.00				
137.05	167.00	164.05	1.00				
138.10	13.00	167.10	5.00				
145.05	1.00	169.05	1.00				
145.80	1.00						

#33: 1-(2,4-DIMETHYLPHENYL)-ETHANONE
Modified: scaled

Entry Number 33 from C:\DATABASE\hjf.l
CAS 000089-74-7
Melting Point -300
Boiling Point -300
Retention Index 66.849
Mol Formula C10H12O
Mol Weight 148.088
Miscellaneous Information
Aldrich: 2', 4'-DIMETHYLACETOPHENONE

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	18.00	39.95	51.00	55.05	28.00	68.05	1.00
26.95	331.00	41.05	122.00	56.00	1.00	70.15	0.00
28.90	26.00	42.05	21.00	57.60	19.00	70.30	0.00
29.90	0.00	43.05	733.00	57.85	13.00	71.00	2.00
33.15	0.00	48.00	1.00	59.00	73.00	72.05	70.00
33.30	0.00	48.95	10.00	61.00	30.00	73.05	165.00

33.60	0.00	49.90	193.00	61.95	121.00	73.95	89.00
35.10	0.00	51.00	681.00	63.05	375.00	75.05	83.00
36.95	19.00	52.00	177.00	64.00	114.00	76.05	98.00
37.95	67.00	53.00	268.00	65.05	337.00	77.05	1765.00
38.90	578.00	54.00	16.00	65.95	70.00	78.05	587.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
79.05	1741.00	91.05	346.00	102.05	158.00	114.00	2.00
80.05	112.00	92.00	29.00	103.05	1253.00	115.05	158.00
81.00	4.00	93.05	11.00	104.05	342.00	116.05	32.00
81.95	0.00	94.05	1.00	105.05	6128.00	117.05	67.00
84.05	2.00	95.00	0.00	106.05	546.00	118.05	24.00
85.00	11.00	95.95	0.00	107.05	22.00	119.05	73.00
86.00	30.00	97.00	3.00	108.05	1.00	120.05	8.00
87.00	33.00	98.00	15.00	109.00	1.00	121.00	1.00
88.00	11.00	99.05	6.00	110.05	2.00	122.00	1.00
89.05	166.00	99.95	0.00	111.05	1.00	123.15	0.00
90.05	58.00	101.05	22.00	113.05	4.00	125.05	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
126.05	5.00	144.10	1.00				
127.05	19.00	145.05	11.00				
128.05	35.00	146.10	7.00				
129.05	21.00	148.15	4248.00				
130.10	4.00	149.15	477.00				
131.05	30.00	150.20	33.00				
133.05	9999.00	151.10	2.00				
134.05	993.00	219.95	0.00				
135.10	62.00						
136.15	3.00						
143.15	1.00						

#34: 2-METHYLPHENOL
Modified: scaled

Entry Number 34 from C:\DATABASE\hjf.l
CAS 000095-48-7
Melting Point -300
Boiling Point -300
Retention Index 59.5
Mol Formula C7H8O
Mol Weight 108.057
Miscellaneous Information
Aldrich: o-cresol

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	107.00	39.90	170.00	54.90	167.00	66.05	146.00
26.95	571.00	41.00	79.00	56.00	7.00	67.00	44.00
28.90	95.00	41.90	36.00	56.95	3.00	68.00	67.00

29.95	4.00	46.95	0.00	57.90	0.00	68.95	4.00
30.90	9.00	47.95	6.00	58.10	1.00	70.00	1.00
33.60	0.00	48.95	67.00	59.95	11.00	71.15	0.00
35.00	0.00	49.95	514.00	60.95	75.00	72.00	3.00
35.95	8.00	50.95	968.00	62.05	174.00	73.00	35.00
36.90	126.00	52.05	516.00	63.05	447.00	74.00	129.00
37.90	288.00	53.05	840.00	64.00	139.00	75.00	65.00
39.00	1094.00	54.00	523.00	65.05	238.00	76.05	62.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
77.05	2758.00	89.05	1227.00	103.05	2.00	128.10	1.00
78.05	629.00	90.05	2233.00	105.05	65.00	129.10	1.00
79.05	3011.00	91.05	633.00	107.05	8088.00	132.00	1.00
80.05	1321.00	92.05	52.00	108.05	9999.00	133.05	0.00
81.05	146.00	93.05	19.00	109.05	782.00	141.05	0.00
82.00	27.00	94.05	3.00	110.05	45.00	144.15	1.00
83.10	2.00	95.00	1.00	111.10	2.00	145.95	0.00
84.00	6.00	95.35	0.00	115.05	1.00	151.20	0.00
85.05	19.00	95.95	0.00	116.05	0.00	152.10	2.00
86.00	29.00	101.00	2.00	121.05	1.00	153.05	0.00
87.00	22.00	102.10	1.00	124.55	0.00	155.05	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
165.15	1.00						
166.20	1.00						
167.15	2.00						
170.10	1.00						
176.05	0.00						
181.00	1.00						
183.10	1.00						

#35: BENZENEETHANOL
Modified: scaled

Entry Number 35 from C:\DATABASE\hjf.l
CAS 000060-12-8
Melting Point -300
Boiling Point -300
Retention Index 60.179
Mol Formula C8H10O
Mol Weight 122.072
Miscellaneous Information
Aldrich: phenethyl alcohol

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	23.00	38.90	665.00	53.05	57.00	64.05	101.00
27.00	119.00	40.00	57.00	53.95	2.00	65.00	1767.00
28.90	70.00	41.05	163.00	54.95	11.00	66.00	116.00
29.95	11.00	42.00	12.00	56.00	1.00	67.00	6.00

30.90	286.00	46.95	1.00	57.00	1.00	68.00	2.00
32.85	2.00	47.85	0.00	58.00	1.00	69.95	0.00
33.75	0.00	48.10	1.00	59.00	7.00	70.85	0.00
34.10	1.00	48.95	18.00	60.00	12.00	71.95	1.00
35.95	1.00	49.90	231.00	60.90	38.00	73.00	12.00
36.95	31.00	50.95	546.00	62.00	114.00	74.00	68.00
37.90	91.00	52.00	136.00	63.00	373.00	75.05	51.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
76.05	50.00	86.00	22.00	98.05	6.00	116.10	0.00
77.05	466.00	87.00	18.00	99.05	2.00	117.10	2.00
78.05	388.00	88.05	3.00	101.00	8.00	118.10	2.00
79.05	91.00	89.05	297.00	102.05	51.00	119.00	6.00
80.05	3.00	91.05	9999.00	103.05	262.00	120.05	35.00
81.05	2.00	92.05	6431.00	104.05	196.00	122.05	2939.00
82.00	0.00	93.05	485.00	105.05	47.00	123.05	255.00
82.80	0.00	94.05	18.00	106.05	4.00	124.10	16.00
83.05	0.00	95.05	2.00	109.90	0.00	125.10	1.00
84.05	2.00	96.00	0.00	114.90	0.00	127.00	0.00
85.00	11.00	97.00	1.00	115.10	1.00	128.10	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
129.15	0.00	166.15	0.00				
132.15	0.00	167.20	0.00				
133.05	0.00	169.05	0.00				
135.10	1.00	180.95	0.00				
141.10	1.00	195.20	2.00				
152.15	0.00						
153.10	1.00						
154.00	0.00						
154.20	0.00						
164.05	0.00						
165.05	1.00						

#36: 1-(3,4-DIMETHYLPHENYL)-ETHANONE
Modified: scaled

Entry Number 36 from C:\DATABASE\hjf.l
CAS 003637-01-2
Melting Point -300
Boiling Point -300
Retention Index 72.689
Mol Formula C10H12O
Mol Weight 148.088
Miscellaneous Information
Aldrich: 3',4'DIMETHYLACETOPHENONE

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	17.00	39.90	47.00	55.00	19.00	68.05	1.00

26.95	312.00	40.95	123.00	55.95	1.00	69.80	0.00
28.90	23.00	42.05	25.00	57.50	13.00	71.00	1.00
32.80	0.00	42.90	735.00	57.80	5.00	72.05	2.00
33.95	0.00	47.80	0.00	59.00	93.00	73.05	19.00
34.60	0.00	49.05	10.00	60.95	26.00	74.00	89.00
35.55	0.00	49.95	207.00	62.00	108.00	75.05	83.00
35.90	0.00	51.05	653.00	63.05	357.00	76.05	92.00
36.90	16.00	52.00	154.00	64.05	86.00	77.05	1713.00
37.90	63.00	53.05	249.00	65.05	306.00	78.05	543.00
38.90	542.00	54.00	15.00	65.90	56.00	79.05	1634.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
80.05	106.00	92.05	23.00	103.05	1196.00	115.05	79.00
81.05	3.00	93.05	7.00	104.05	313.00	116.05	16.00
81.90	0.00	94.00	0.00	105.05	5425.00	117.05	33.00
84.00	1.00	95.05	0.00	106.05	480.00	118.05	15.00
85.00	9.00	96.05	0.00	107.05	17.00	119.05	88.00
86.00	25.00	97.00	3.00	108.05	0.00	120.10	9.00
87.05	28.00	98.00	18.00	109.00	1.00	121.05	1.00
88.00	9.00	99.00	6.00	110.05	1.00	122.10	0.00
89.05	163.00	100.00	0.00	111.05	1.00	123.05	0.00
90.05	60.00	101.05	19.00	113.05	2.00	123.15	0.00
91.05	272.00	102.05	149.00	114.00	2.00	123.30	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
124.05	0.00	137.05	1.00	211.20	0.00		
126.05	3.00	143.10	1.00				
127.05	7.00	144.20	0.00				
128.10	12.00	145.15	3.00				
129.05	5.00	146.15	6.00				
130.10	1.00	148.20	4124.00				
131.05	64.00	149.20	458.00				
133.05	9999.00	150.15	33.00				
134.05	1007.00	151.10	2.00				
135.05	61.00	152.05	0.00				
136.10	3.00	155.05	0.00				

#37: 2,6-DIMETHYL-4-NITROPHENOL
Modified: scaled

Entry Number 37 from C:\DATABASE\hjf.l
CAS 002423-71-4
Melting Point -300
Boiling Point -300
Retention Index 89.31
Mol Formula C8H9NO3
Mol Weight 167.057

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.

25.95	60.00	38.90	1429.00	51.00	1003.00	63.00	605.00
27.00	543.00	40.00	247.00	52.05	436.00	64.05	200.00
28.90	88.00	41.05	742.00	53.05	1549.00	65.05	1547.00
29.90	323.00	42.05	64.00	54.05	113.00	66.05	318.00
32.95	0.00	43.00	717.00	55.05	431.00	67.05	587.00
33.90	1.00	45.90	24.00	56.05	26.00	68.05	106.00
34.90	1.00	46.80	2.00	57.05	12.00	69.00	180.00
35.15	0.00	47.05	2.00	58.95	13.00	70.05	13.00
35.95	2.00	47.90	3.00	59.95	6.00	71.05	3.00
36.90	66.00	48.95	26.00	60.90	73.00	72.05	0.00
37.90	206.00	49.90	346.00	62.05	237.00	73.00	18.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
74.05	115.00	85.05	27.00	97.05	4.00	108.05	122.00
75.05	119.00	86.05	57.00	98.05	12.00	109.05	556.00
76.00	75.00	87.05	53.00	99.05	6.00	110.05	44.00
77.05	5798.00	88.05	14.00	100.05	0.00	111.10	4.00
78.05	844.00	89.05	184.00	101.05	26.00	112.10	1.00
79.05	681.00	91.05	5130.00	102.05	144.00	113.10	0.00
80.05	107.00	92.05	531.00	103.05	505.00	114.05	0.00
81.05	1063.00	93.05	758.00	104.05	59.00	115.05	1.00
82.05	81.00	94.05	272.00	105.05	74.00	116.05	11.00
83.05	18.00	95.05	78.00	106.05	60.00	117.05	6.00
84.00	7.00	96.05	20.00	107.05	127.00	118.05	24.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
119.05	248.00	130.05	1.00	143.05	0.00	155.20	0.00
120.05	463.00	132.05	5.00	145.20	1.00	159.20	1.00
121.05	919.00	133.05	2.00	146.10	1.00	160.15	1.00
122.05	145.00	134.05	47.00	147.05	2.00	162.15	2.00
123.05	17.00	135.05	54.00	148.15	2.00	163.10	2.00
124.05	3.00	136.15	96.00	149.20	6.00	164.05	14.00
125.10	1.00	137.05	2946.00	150.05	120.00	165.05	21.00
126.15	0.00	138.05	267.00	151.10	342.00	166.20	74.00
127.10	1.00	139.20	23.00	152.05	53.00	167.05	9999.00
128.10	1.00	140.05	2.00	153.10	6.00	168.05	1083.00
129.10	2.00	141.10	0.00	154.20	0.00	169.05	114.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
170.15	8.00	193.05	1.00				
171.15	1.00	194.20	0.00				
175.20	1.00	196.20	1.00				
178.10	0.00	198.20	1.00				
179.10	1.00	205.20	0.00				
181.05	1.00	207.05	1.00				
182.30	0.00	209.05	0.00				
183.20	1.00	220.10	0.00				
186.05	1.00						
189.20	1.00						
191.15	0.00						

#38: 3-ACETYL-2,5-DIMETHYLFURAN
Modified: scaled
Entry Number 38 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 54.219
Mol Formula C8H10O2
Mol Weight 138.068

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	48.00	39.90	67.00	54.95	61.00	66.00	54.00
26.90	266.00	41.00	276.00	56.00	4.00	67.05	353.00
28.95	26.00	42.00	186.00	57.00	2.00	68.05	28.00
29.90	1.00	42.90	6916.00	57.65	0.00	69.00	156.00
30.95	4.00	47.50	32.00	58.00	1.00	70.95	1.00
32.85	2.00	48.95	42.00	58.95	3.00	71.75	1.00
34.75	1.00	49.90	328.00	60.05	1.00	72.05	0.00
35.95	2.00	50.90	441.00	61.00	131.00	73.00	7.00
36.85	38.00	52.00	345.00	63.00	79.00	74.05	28.00
37.90	78.00	53.00	1316.00	64.00	19.00	75.05	12.00
38.95	366.00	54.00	79.00	65.05	185.00	76.05	8.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
77.05	103.00	87.15	0.00	97.05	7.00	110.10	8.00
78.00	30.00	87.30	0.00	98.05	1.00	111.10	2.00
79.00	110.00	88.15	0.00	99.15	0.00	112.05	0.00
80.00	70.00	89.05	3.00	101.30	0.00	118.05	2.00
81.05	3312.00	90.05	3.00	102.05	0.00	119.00	59.00
82.05	185.00	91.05	44.00	103.05	0.00	120.05	14.00
83.05	12.00	92.05	9.00	105.00	15.00	121.05	26.00
84.00	2.00	93.05	34.00	106.10	2.00	122.05	188.00
85.05	2.00	94.05	209.00	107.05	8.00	123.05	9999.00
85.95	1.00	95.05	881.00	108.05	15.00	124.05	760.00
87.05	0.00	96.05	89.00	109.05	84.00	125.05	63.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
126.05	4.00	150.05	0.00				
129.90	0.00	176.20	0.00				
135.05	6.00	220.05	0.00				
136.05	28.00						
137.05	234.00						
138.05	6036.00						
139.10	542.00						
140.05	46.00						
141.10	3.00						
147.20	0.00						
148.05	0.00						

#39: 1-(3-METHYLPHENYL)-ETHANONE
Modified: scaled
Entry Number 39 from C:\DATABASE\hjf.l
CAS 000585-74-0
Melting Point -300
Boiling Point -300
Retention Index 62.31
Mol Formula C9H10O
Mol Weight 134.073
Miscellaneous Information
Aldrich: 3'-
methylacetophenone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	19.00	39.95	71.00	53.05	71.00	65.05	1993.00
26.95	125.00	41.05	199.00	54.05	3.00	66.05	119.00
28.90	4.00	42.05	41.00	55.05	7.00	67.00	7.00
33.30	0.00	43.00	1165.00	55.80	1.00	67.95	0.00
34.40	0.00	44.95	55.00	56.10	0.00	70.65	0.00
34.65	0.00	46.75	1.00	57.45	7.00	71.15	0.00
35.05	0.00	47.95	1.00	59.05	114.00	72.00	1.00
35.95	1.00	48.95	18.00	60.90	65.00	73.00	18.00
36.90	36.00	49.90	249.00	62.05	220.00	74.05	88.00
37.90	117.00	51.00	444.00	63.05	655.00	75.05	68.00
38.90	881.00	52.05	101.00	64.05	180.00	76.05	55.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
77.05	221.00	89.05	653.00	102.05	21.00	115.05	31.00
78.05	62.00	90.05	311.00	103.05	71.00	116.05	5.00
79.05	65.00	91.05	8499.00	104.05	25.00	117.05	22.00
80.05	4.00	92.05	691.00	105.05	48.00	119.05	9999.00
80.95	1.00	93.05	25.00	106.10	4.00	120.05	902.00
82.05	0.00	94.05	1.00	107.10	1.00	121.05	54.00
84.00	5.00	96.15	0.00	109.05	3.00	122.05	3.00
85.00	26.00	97.05	3.00	110.10	2.00	128.15	0.00
86.05	57.00	98.00	7.00	111.05	1.00	131.05	7.00
87.00	47.00	99.00	1.00	113.05	3.00	132.05	7.00
88.10	17.00	101.00	4.00	114.00	2.00	133.15	66.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
134.05	3949.00						
135.05	418.00						
136.10	28.00						
137.10	2.00						
138.15	0.00						
147.15	1.00						
148.05	0.00						
206.95	0.00						

#40: 1,2-BENZENEDICARBOXYLIC ACID
Modified: scaled
Entry Number 40 from C:\DATABASE\hjf.l
CAS 000088-99-3
Melting Point -300
Boiling Point -300
Retention Index 79.23
Mol Formula C8H6O4
Mol Weight 166.026
Miscellaneous Information
Aldrich: phthalic acid

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	71.00	40.95	3.00	57.00	1.00	67.90	2.00
28.90	14.00	42.15	3.00	57.80	2.00	70.40	1.00
30.00	0.00	47.90	57.00	59.85	58.00	72.00	41.00
31.00	27.00	48.90	465.00	60.95	169.00	72.95	427.00
33.75	2.00	49.95	4870.00	61.95	108.00	74.05	1733.00
34.55	1.00	50.95	306.00	63.00	108.00	75.05	1181.00
36.00	84.00	51.95	672.00	64.00	34.00	76.05	8971.00
36.95	829.00	52.90	155.00	64.95	25.00	77.05	746.00
37.90	1254.00	54.00	5.00	65.95	46.00	78.05	30.00
38.90	132.00	54.65	1.00	66.85	1.00	79.00	4.00
39.90	3.00	56.10	3.00	67.15	1.00	81.40	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
81.90	1.00	93.00	4.00	122.30	1.00	181.20	1.00
83.15	1.00	94.05	1.00	132.00	1.00	196.15	6.00
83.95	15.00	101.00	12.00	134.05	2.00		
85.00	15.00	102.05	6.00	148.05	3061.00		
86.00	13.00	104.05	9999.00	149.05	278.00		
87.05	4.00	105.05	782.00	150.00	28.00		
89.00	1.00	106.05	46.00	150.95	1.00		
89.30	1.00	107.05	4.00	151.05	1.00		
90.00	4.00	111.90	1.00	151.20	1.00		
91.05	5.00	119.05	1.00	168.10	3.00		
92.05	14.00	120.00	1.00	170.10	5.00		

#41: 1,4-DIMETHOXYBENZENE
Modified: scaled
Entry Number 41 from C:\DATABASE\hjf.l
CAS 000150-78-7
Melting Point -300
Boiling Point -300
Retention Index 60.189
Mol Formula C8H10O2
Mol Weight 138.068

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	226.00	41.00	1102.00	56.00	5.00	68.90	131.00
26.90	85.00	42.00	47.00	57.00	2.00	70.95	1.00
28.90	61.00	46.95	0.00	58.90	3.00	71.05	0.00
29.90	8.00	47.95	1.00	59.95	6.00	71.80	0.00
30.95	13.00	48.90	21.00	60.90	68.00	72.05	0.00
34.15	0.00	49.90	283.00	62.00	197.00	72.95	19.00
35.90	2.00	50.90	403.00	63.00	691.00	73.95	102.00
36.90	61.00	52.00	554.00	64.05	733.00	75.00	52.00
37.90	245.00	52.90	373.00	65.05	657.00	76.05	61.00
38.90	382.00	53.90	369.00	66.05	117.00	77.05	454.00
40.00	33.00	54.90	73.00	67.05	208.00	78.05	62.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
79.05	248.00	90.00	1.00	104.05	0.00	117.05	0.00
80.05	470.00	91.05	1.00	105.05	8.00	120.05	1.00
81.05	36.00	92.05	411.00	106.10	0.00	121.10	1.00
82.00	105.00	93.05	38.00	107.00	166.00	123.05	9999.00
82.95	5.00	94.00	35.00	108.05	165.00	124.05	775.00
84.00	1.00	95.05	2993.00	109.05	40.00	125.05	63.00
85.00	5.00	96.05	191.00	110.05	7.00	126.05	4.00
85.95	1.00	97.00	11.00	111.05	1.00	135.05	16.00
87.15	0.00	97.85	0.00	112.05	0.00	136.25	2.00
89.05	0.00	98.10	1.00	112.65	0.00	138.05	8163.00
89.30	0.00	102.90	0.00	114.10	1.00	139.05	699.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
140.05	57.00						
141.15	4.00						
151.10	0.00						
152.05	0.00						
161.10	0.00						
164.05	0.00						
176.05	1.00						
230.20	0.00						

#42: 1-(2-HYDROXY-5-METHYLPHENYL)-ETHANONE
Modified: scaled
Entry Number 42 from C:\DATABASE\hjf.l
CAS 001450-72-2
Melting Point -300
Boiling Point -300
Retention Index 69.599
Mol Formula C9H10O2
Mol Weight 150.068
Miscellaneous Information
Aldrich: 2'-hydroxy-5'-methylacetophenone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	39.00	37.90	82.00	50.90	612.00	63.00	224.00
26.90	268.00	38.90	454.00	52.05	287.00	64.00	50.00
28.90	54.00	39.90	47.00	52.95	567.00	65.05	119.00
29.90	2.00	40.90	68.00	53.80	43.00	66.00	58.00
30.95	9.00	42.00	44.00	54.95	132.00	67.05	230.00
32.95	1.00	42.90	1063.00	56.00	5.00	68.90	4.00
34.10	0.00	45.90	2.00	57.00	3.00	70.00	1.00
34.65	0.00	46.95	7.00	58.90	15.00	71.05	1.00
34.95	1.00	47.95	3.00	60.05	22.00	71.95	1.00
35.90	2.00	48.95	22.00	61.00	61.00	73.00	13.00
36.90	28.00	49.90	233.00	62.00	89.00	74.05	80.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
75.05	128.00	86.05	16.00	97.00	1.00	109.00	12.00
76.00	56.00	87.05	16.00	98.05	4.00	110.10	1.00
77.05	1950.00	88.05	7.00	99.05	1.00	111.10	0.00
78.05	453.00	89.00	68.00	101.05	8.00	113.05	1.00
79.05	669.00	90.05	32.00	102.00	29.00	114.00	0.00
80.05	55.00	91.05	152.00	103.05	111.00	115.05	2.00
81.00	33.00	92.05	23.00	104.00	65.00	116.10	1.00
82.00	4.00	93.05	36.00	105.05	177.00	117.05	1.00
83.00	1.00	94.05	6.00	106.00	116.00	118.05	3.00
84.05	2.00	95.05	3.00	107.05	2278.00	119.05	9.00
85.05	8.00	96.00	1.00	108.05	199.00	120.05	6.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
121.05	42.00	138.05	4.00	153.10	3.00		
122.05	5.00	139.10	0.00	159.20	0.00		
123.05	0.00	141.15	1.00	161.10	1.00		
128.30	0.00	142.20	1.00	165.20	0.00		
129.05	1.00	145.05	0.00	176.20	0.00		
131.05	262.00	146.20	0.00	209.20	1.00		
132.05	74.00	147.05	5.00				
133.05	19.00	148.05	20.00				
135.05	9999.00	150.05	5591.00				
136.05	873.00	151.05	532.00				
137.05	69.00	152.10	43.00				

#43: 1-(4-HYDROXY-3-NITROPHENYL)-ETHANONE
Modified: scaled

Entry Number 43 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 84.39
Mol Formula C8H7NO4
Mol Weight 181.037
Miscellaneous Information
Aldrich: 4'-hydroxy-3'-nitroacetophenone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	35.00	39.90	18.00	53.90	38.00	68.05	9.00
26.95	72.00	40.95	20.00	54.95	46.00	70.05	4.00
28.90	32.00	42.05	74.00	56.05	1.00	72.05	1.00
29.90	109.00	42.90	2253.00	60.00	11.00	73.00	20.00
30.90	2.00	46.90	2.00	61.00	109.00	74.05	75.00
32.95	1.00	48.00	5.00	62.00	357.00	75.00	73.00
33.90	0.00	48.90	30.00	63.00	866.00	76.05	65.00
35.90	1.00	49.90	202.00	64.05	409.00	77.05	334.00
36.85	83.00	50.95	358.00	65.05	158.00	78.05	97.00
37.90	205.00	52.00	188.00	66.00	74.00	79.05	134.00
38.95	275.00	52.90	619.00	67.05	32.00	80.05	100.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
81.00	17.00	92.05	1021.00	105.05	49.00	117.05	3.00
82.05	4.00	93.05	192.00	106.05	64.00	118.05	12.00
83.05	3.00	94.05	41.00	107.05	61.00	119.05	225.00
84.05	3.00	95.05	9.00	108.05	408.00	120.05	5037.00
85.05	0.00	96.05	1.00	109.05	31.00	121.05	429.00
86.00	11.00	98.05	2.00	110.05	5.00	122.05	46.00
87.05	9.00	99.10	1.00	111.10	0.00	123.05	6.00
88.05	5.00	100.95	2.00	113.10	3.00	124.05	1.00
89.00	28.00	102.05	2.00	114.05	0.00	125.10	1.00
90.00	28.00	103.05	5.00	115.10	2.00	127.15	2.00
91.05	492.00	104.05	11.00	116.05	1.00	128.15	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
129.05	0.00	142.20	0.00	154.10	1.00	168.05	115.00
130.05	0.00	144.20	0.00	155.20	2.00	169.05	10.00
131.05	0.00	145.00	1.00	156.20	0.00	170.10	1.00
132.05	1.00	146.05	6.00	159.05	0.00	177.05	1.00
133.05	5.00	147.10	3.00	160.15	1.00	178.15	1.00
134.05	12.00	148.05	17.00	161.10	2.00	179.15	4.00
135.05	28.00	149.05	217.00	162.05	1.00	181.05	2719.00
136.05	142.00	150.05	125.00	163.05	2.00	182.05	275.00
137.05	13.00	151.05	46.00	164.05	8.00	183.05	34.00
138.05	12.00	152.05	16.00	166.05	9999.00	184.10	3.00

139.05	4.00	153.05	2.00	167.05	841.00	193.20	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
194.15	2.00						
207.05	0.00						
210.25	1.00						
211.25	1.00						
220.20	0.00						
224.30	2.00						
225.30	2.00						
226.20	0.00						

#44: A-METHYLBENZENE METHANOL
Modified: scaled

Entry Number 44 from C:\DATABASE\hjf.l
CAS 000098-85-1
Melting Point -300
Boiling Point -300
Retention Index 55.77
Mol Formula C8H10O
Mol Weight 122.072
Miscellaneous Information
Aldrich: sec-phenethyl alcohol

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	46.00	38.90	585.00	51.95	465.00	65.05	193.00
26.95	379.00	39.90	50.00	53.40	672.00	66.00	30.00
28.90	197.00	40.95	55.00	54.90	32.00	67.00	8.00
29.90	4.00	42.90	2747.00	55.95	2.00	67.95	5.00
33.00	0.00	44.90	272.00	56.95	1.00	69.95	0.00
33.40	0.00	45.90	3.00	59.00	15.00	70.30	0.00
34.10	1.00	46.90	3.00	60.00	103.00	71.15	0.00
34.60	1.00	48.00	3.00	60.90	48.00	71.30	0.00
35.95	3.00	48.95	52.00	61.90	119.00	72.00	2.00
36.95	50.00	49.90	680.00	62.90	283.00	72.90	42.00
37.95	138.00	50.90	1863.00	64.00	50.00	73.90	230.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
74.95	147.00	85.95	19.00	97.00	4.00	110.05	3.00
76.00	198.00	87.00	20.00	98.00	15.00	114.80	0.00
77.05	4584.00	87.95	5.00	98.95	5.00	115.10	0.00
78.05	1965.00	89.05	89.00	101.00	15.00	117.05	0.00
79.05	8859.00	90.00	19.00	102.05	113.00	118.05	2.00
80.05	589.00	91.05	252.00	103.05	453.00	118.95	2.00
81.00	22.00	92.05	23.00	104.05	394.00	120.05	56.00
81.95	2.00	93.00	37.00	105.05	1060.00	121.05	488.00
83.00	0.00	94.05	8.00	107.05	9999.00	122.05	3541.00
83.90	3.00	94.95	3.00	108.05	753.00	123.05	299.00

85.00	10.00	95.95	1.00	109.00	46.00	124.05	20.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
125.05	1.00	219.95	0.00				
127.15	0.00						
128.05	1.00						
129.05	1.00						
133.05	0.00						
155.10	4.00						
155.95	0.00						
163.95	0.00						
166.05	0.00						
181.00	1.00						
211.05	2.00						

#45: 3-METHYBENZENE METHANOL
Modified: scaled

Entry Number 45 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 61.909
Mol Formula C8H10O
Mol Weight 122.072
Miscellaneous Information
Aldrich: 3-
methylbenzylalcohol

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	49.00	39.90	165.00	51.90	318.00	65.00	1828.00
26.90	470.00	40.95	377.00	52.95	368.00	66.00	188.00
28.90	228.00	41.95	27.00	53.90	30.00	67.00	39.00
29.95	18.00	44.90	43.00	54.90	87.00	68.00	11.00
30.90	183.00	45.90	56.00	55.95	4.00	69.95	1.00
32.95	2.00	46.90	17.00	56.95	5.00	70.90	1.00
33.95	0.00	47.75	5.00	58.95	82.00	71.10	0.00
35.95	2.00	48.00	0.00	60.05	722.00	71.90	2.00
36.90	73.00	48.95	39.00	61.90	309.00	72.90	24.00
37.90	222.00	49.90	461.00	62.90	824.00	73.95	142.00
38.90	1500.00	50.90	1174.00	64.00	185.00	75.00	107.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
76.00	126.00	87.00	54.00	96.95	4.00	109.95	2.00
77.05	4568.00	88.00	14.00	97.95	15.00	111.15	0.00
78.05	1122.00	89.05	456.00	98.95	4.00	115.05	1.00
79.05	5253.00	90.05	145.00	101.00	14.00	116.05	2.00
80.05	349.00	91.05	5278.00	102.05	119.00	117.05	3.00
81.00	32.00	92.05	554.00	103.05	777.00	118.05	3.00

81.95	5.00	93.05	4772.00	104.05	1541.00	119.05	457.00
83.00	1.00	94.05	385.00	105.05	1095.00	120.05	216.00
84.00	9.00	95.00	21.00	107.05	7405.00	121.05	1504.00
84.95	34.00	95.95	2.00	108.05	562.00	122.05	9999.00
85.95	67.00	96.10	0.00	109.00	34.00	123.05	850.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
124.05	55.00	153.05	1.00				
125.05	4.00	154.10	2.00				
127.30	0.00	167.05	0.00				
128.10	2.00	169.00	4.00				
129.10	2.00	170.15	1.00				
132.00	0.00	181.00	1.00				
132.95	0.00	183.15	1.00				
134.05	0.00						
141.15	1.00						
142.05	1.00						
152.05	0.00						

#46: 2-ISOPROPYLPHENOL
Modified: scaled

Entry Number 46 from C:\DATABASE\hjf.l
CAS 000088-69-7
Melting Point -300
Boiling Point -300
Retention Index 68.42
Mol Formula C9H12O
Mol Weight 136.088

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	25.00	40.90	270.00	54.90	136.00	70.00	1.00
26.90	227.00	41.95	22.00	56.00	6.00	71.00	0.00
28.90	44.00	44.95	42.00	57.35	27.00	72.15	0.00
29.90	0.00	45.85	53.00	59.00	59.00	72.95	6.00
32.95	1.00	47.85	1.00	60.40	174.00	73.90	52.00
34.10	0.00	48.95	9.00	61.90	76.00	74.90	95.00
36.00	1.00	49.90	140.00	62.90	234.00	76.05	73.00
36.90	23.00	50.90	478.00	64.05	76.00	77.00	1696.00
37.90	90.00	51.90	114.00	65.00	488.00	78.05	219.00
38.90	645.00	52.90	192.00	66.00	157.00	79.05	135.00
39.90	88.00	53.90	19.00	67.00	175.00	80.00	11.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
81.00	16.00	92.05	175.00	104.05	178.00	115.05	240.00
81.95	2.00	93.05	809.00	105.05	52.00	116.05	49.00
83.00	1.00	94.05	149.00	106.05	7.00	117.05	57.00
84.00	1.00	95.05	95.00	107.05	279.00	118.00	23.00
84.95	5.00	96.05	6.00	108.05	26.00	119.05	129.00

85.95	12.00	97.00	1.00	109.05	4.00	121.05	9999.00
86.95	14.00	98.00	6.00	109.95	1.00	122.05	907.00
88.05	6.00	99.05	2.00	111.05	1.00	123.05	58.00
89.05	123.00	101.05	48.00	111.95	0.00	124.05	3.00
90.05	45.00	102.05	215.00	113.05	3.00	127.10	0.00
91.05	1479.00	103.05	2024.00	114.00	2.00	128.10	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
129.05	0.00	145.05	0.00				
131.00	5.00	146.95	0.00				
132.05	1.00	150.00	0.00				
133.05	10.00	150.20	0.00				
134.05	9.00	153.05	1.00				
136.05	4058.00	154.05	0.00				
137.05	399.00	155.20	0.00				
138.05	26.00	165.20	0.00				
139.15	2.00	171.05	2.00				
141.10	1.00	172.05	0.00				
142.10	1.00						

#47: 2,3-DIMETHOXYTOLUENE
Modified: scaled

Entry Number 47 from C:\DATABASE\hjf.l
CAS 004463-33-6
Melting Point -300
Boiling Point -300
Retention Index 59.84
Mol Formula C9H12O2
Mol Weight 152.082

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	53.00	38.90	1060.00	53.90	54.00	64.00	127.00
26.90	174.00	39.90	357.00	54.90	169.00	64.95	1269.00
28.90	50.00	40.90	262.00	55.95	8.00	66.00	1066.00
29.95	7.00	41.95	22.00	57.00	6.00	67.00	111.00
30.90	33.00	46.90	30.00	57.60	0.00	68.00	29.00
32.85	36.00	47.80	0.00	57.85	1.00	68.90	24.00
34.30	0.00	48.90	18.00	58.95	6.00	69.95	1.00
35.10	0.00	49.90	248.00	59.90	3.00	70.90	1.00
35.85	0.00	50.90	608.00	60.90	35.00	71.55	0.00
36.90	44.00	51.90	321.00	61.90	109.00	71.90	0.00
37.90	149.00	52.95	498.00	62.90	317.00	72.95	8.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
73.90	54.00	84.90	5.00	96.05	8.00	110.05	255.00
74.90	37.00	86.00	12.00	97.10	1.00	111.05	15.00
76.00	80.00	86.95	9.00	100.90	1.00	112.05	2.00
77.00	1693.00	88.05	1.00	102.05	3.00	117.10	1.00

78.05	456.00	89.00	147.00	103.05	6.00	118.05	7.00
79.05	1448.00	90.00	88.00	104.05	2.00	119.00	28.00
80.05	115.00	91.05	2312.00	105.00	240.00	120.05	9.00
81.05	1126.00	92.05	217.00	106.05	116.00	121.05	114.00
82.05	72.00	93.00	213.00	107.05	605.00	122.00	371.00
83.05	8.00	94.05	1400.00	108.05	105.00	123.00	41.00
83.95	2.00	95.00	112.00	109.05	3304.00	124.05	5.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
125.10	1.00	150.10	1.00				
131.95	1.00	152.05	9999.00				
133.05	3.00	153.05	979.00				
134.05	1.00	154.05	82.00				
135.05	149.00	155.10	5.00				
136.05	262.00	197.95	0.00				
137.05	5195.00	214.10	2.00				
138.05	460.00	228.15	1.00				
139.05	37.00						
140.05	3.00						
149.05	3.00						

#48: 3-METHOXYACETOPHENONE
Modified: scaled

Entry Number 48 from C:\DATABASE\hjf.l
CAS 000586-37-8
Melting Point -300
Boiling Point -300
Retention Index 72.579
Mol Formula C9H10O2
Mol Weight 150.068

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	19.00	37.90	236.00	51.90	107.00	61.90	176.00
26.90	81.00	38.90	324.00	52.90	137.00	62.90	870.00
28.90	17.00	39.90	15.00	53.90	9.00	64.00	1041.00
29.90	0.00	40.95	25.00	54.95	14.00	64.95	332.00
33.55	0.00	42.00	50.00	56.00	2.00	65.95	53.00
33.85	0.00	42.90	1605.00	56.95	1.00	67.05	18.00
34.15	0.00	47.85	1.00	57.75	0.00	67.35	3.00
34.65	0.00	48.05	0.00	58.30	0.00	70.55	0.00
34.95	0.00	48.90	25.00	59.00	2.00	71.15	0.00
35.95	2.00	49.90	420.00	59.95	5.00	71.95	1.00
36.90	52.00	50.90	401.00	60.90	56.00	72.95	25.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
73.90	161.00	84.95	7.00	96.00	0.00	107.05	4604.00
74.95	127.00	85.95	12.00	96.80	0.00	108.05	381.00

76.00	351.00	87.00	9.00	96.90	0.00	109.05	23.00
77.05	3318.00	88.00	4.00	97.05	0.00	110.10	2.00
78.05	452.00	89.00	58.00	97.95	4.00	115.05	2.00
79.05	246.00	90.05	19.00	99.05	2.00	116.05	2.00
80.05	17.00	91.05	225.00	101.05	3.00	117.00	2.00
81.00	3.00	92.05	1577.00	102.00	7.00	118.05	5.00
81.95	1.00	93.00	139.00	103.05	22.00	119.00	52.00
83.05	0.00	94.00	8.00	104.05	35.00	120.05	41.00
83.95	1.00	95.00	1.00	105.05	96.00	121.05	45.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.00	6.00	136.05	871.00	169.00	0.00		
123.05	0.00	137.05	68.00	199.20	0.00		
124.05	0.00	138.05	5.00	215.10	1.00		
124.90	0.00	146.95	0.00				
125.10	1.00	147.05	0.00				
127.15	0.00	147.20	0.00				
127.90	0.00	148.05	50.00				
128.15	0.00	150.05	6178.00				
132.00	0.00	151.05	604.00				
133.05	161.00	152.05	50.00				
135.05	9999.00	153.05	3.00				

#49: 4-METHYL-1,2-BENZENEDICARBOXYLIC ACID
Modified: scaled

Entry Number 49 from C:\DATABASE\hjf.l
CAS 004316-23-8
Melting Point -300
Boiling Point -300
Retention Index 83.84
Mol Formula C9H8O4
Mol Weight 180.042
Miscellaneous Information
Aldrich: 4-methylphthalic acid

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	55.00	37.90	366.00	50.90	590.00	62.90	2521.00
26.90	121.00	38.90	1042.00	51.90	71.00	64.05	837.00
27.90	15.00	39.90	227.00	52.90	113.00	64.95	63.00
28.90	5.00	40.90	9.00	53.90	5.00	65.90	16.00
30.90	7.00	42.90	598.00	55.65	1.00	67.00	1.00
32.80	1.00	43.90	198.00	56.90	10.00	71.95	9.00
33.40	1.00	44.90	782.00	58.05	34.00	72.90	103.00
33.80	1.00	46.95	1.00	58.90	91.00	73.90	382.00
34.10	0.00	47.90	19.00	59.90	56.00	74.95	293.00
35.95	19.00	48.90	138.00	60.90	395.00	75.95	54.00
36.90	252.00	49.90	779.00	61.90	1006.00	76.90	92.00

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
78.00	19.00	91.05	469.00	106.00	5.00	121.00	2.00
78.95	6.00	92.05	19.00	107.05	1.00	126.05	1.00
79.95	0.00	93.00	1.00	109.05	1.00	132.00	35.00
82.40	1.00	93.95	1.00	111.05	1.00	133.00	6.00
83.95	48.00	97.00	4.00	113.00	0.00	134.05	1.00
84.95	163.00	98.00	5.00	114.90	1.00	135.05	2.00
86.00	287.00	100.95	8.00	115.10	2.00	139.00	1.00
87.00	230.00	102.00	2.00	116.05	1.00	143.05	1.00
88.05	118.00	103.00	8.00	118.05	9999.00	146.05	4.00
89.05	4914.00	104.05	16.00	119.05	898.00	147.05	2.00
90.05	6204.00	105.00	10.00	120.00	54.00	160.05	13.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
161.00	73.00						
162.05	4024.00						
163.05	457.00						
164.05	45.00						
165.05	6.00						
166.05	1.00						
181.05	1.00						
207.00	0.00						
224.05	10.00						
225.05	1.00						
237.05	4.00						

#50: 2,5-DIMETHYLPHENOL
Modified: scaled

Entry Number 50 from C:\DATABASE\hjf.l
CAS 000095-87-4
Melting Point -300
Boiling Point -300
Retention Index 65.12
Mol Formula C8H10O
Mol Weight 122.072

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	52.00	43.05	70.00	54.90	178.00	66.95	120.00
26.90	478.00	44.90	51.00	55.95	7.00	68.05	20.00
32.95	1.00	45.90	74.00	56.90	3.00	68.90	2.00
35.05	0.00	46.90	16.00	59.00	82.00	69.90	1.00
35.95	2.00	47.85	5.00	60.00	394.00	71.95	1.00
36.90	51.00	49.00	31.00	60.90	196.00	72.90	16.00
37.90	157.00	49.90	333.00	61.90	123.00	73.90	89.00
38.90	921.00	50.90	849.00	62.90	307.00	74.95	67.00
39.90	134.00	51.90	310.00	63.95	75.00	76.00	71.00
40.90	315.00	52.90	565.00	65.00	602.00	77.00	2499.00

41.90	34.00	53.90	64.00	65.95	147.00	78.00	864.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
79.05	1649.00	90.05	7.00	102.05	97.00	121.05	3750.00
80.05	153.00	91.05	1694.00	103.05	703.00	122.05	9999.00
81.00	62.00	92.00	210.00	104.00	611.00	123.05	879.00
82.05	35.00	93.00	473.00	105.05	327.00	124.05	55.00
83.00	5.00	94.05	332.00	107.05	9394.00	125.10	2.00
84.00	4.00	95.00	46.00	108.05	738.00	128.15	1.00
84.95	13.00	96.00	6.00	109.05	45.00	128.90	0.00
85.95	27.00	97.00	3.00	110.05	3.00	131.90	1.00
86.95	22.00	98.00	8.00	117.00	1.00	133.00	1.00
88.00	5.00	99.00	3.00	118.05	4.00	135.00	1.00
89.00	92.00	101.00	15.00	119.00	46.00	150.00	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
165.05	1.00						
166.05	2.00						
184.20	0.00						

#51: 1-NITRO-2,5-DIMETHYLBENZENE
Modified: scaled

Entry Number 51 from C:\DATABASE\hjf.l
CAS 000089-87-2
Melting Point -300
Boiling Point -300
Retention Index 70.989
Mol Formula C8H9NO2
Mol Weight 151.062
Miscellaneous Information
Aldrich: 4-nitro-m-xylene

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	56.00	48.05	2.00	60.05	10.00	72.00	1.00
26.90	810.00	48.90	33.00	60.90	88.00	72.95	26.00
29.90	180.00	49.90	517.00	61.90	303.00	73.95	179.00
35.90	1.00	50.90	1422.00	62.90	925.00	74.90	172.00
36.90	65.00	51.90	496.00	64.00	231.00	76.05	242.00
37.90	197.00	52.90	779.00	64.95	867.00	77.05	6435.00
38.90	1480.00	54.00	72.00	66.05	239.00	78.05	1893.00
39.90	139.00	54.95	68.00	67.00	74.00	79.05	7737.00
40.90	269.00	55.95	5.00	67.95	12.00	80.05	597.00
42.00	23.00	56.95	1.00	70.00	1.00	81.00	35.00
46.90	5.00	58.50	4.00	70.95	1.00	82.05	6.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
83.00	3.00	94.05	40.00	105.05	1072.00	119.00	40.00
83.95	5.00	95.00	12.00	106.05	2973.00	120.05	92.00
84.95	23.00	96.10	3.00	107.05	702.00	121.05	131.00

85.95	60.00	96.95	7.00	108.00	55.00	122.05	31.00
86.95	60.00	98.00	28.00	109.05	3.00	123.05	4.00
88.00	18.00	98.95	11.00	110.95	2.00	123.90	0.00
89.05	394.00	99.95	1.00	113.95	0.00	124.15	0.00
90.00	111.00	101.05	36.00	115.05	1.00	128.15	0.00
91.05	992.00	102.05	340.00	116.05	53.00	130.05	2.00
92.05	248.00	103.05	2381.00	117.05	22.00	132.05	24.00
93.05	127.00	104.05	959.00	118.05	32.00	134.05	9999.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
135.05	976.00	154.10	2.00				
136.05	67.00	167.05	0.00				
137.05	5.00	182.15	1.00				
145.00	1.00						
146.15	2.00						
147.05	2.00						
148.15	1.00						
149.05	10.00						
151.05	1845.00						
152.05	218.00						
153.05	18.00						

#52: 2-METHYLBENZOIC ACID
Modified: scaled

Entry Number 52 from C:\DATABASE\hjf.l
CAS 000118-90-1
Melting Point -300
Boiling Point -300
Retention Index 73.129
Mol Formula C8H8O2
Mol Weight 136.051
Miscellaneous Information
Aldrich: o-toluic acid

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	46.00	44.90	647.00	54.95	49.00	66.95	36.00
26.95	252.00	45.75	21.00	56.05	5.00	68.00	14.00
34.10	5.00	46.65	1.00	56.95	8.00	70.00	1.00
35.05	2.00	46.80	1.00	58.00	3.00	71.00	7.00
35.90	12.00	47.90	7.00	58.95	790.00	71.95	5.00
36.90	121.00	48.90	58.00	60.90	180.00	72.95	38.00
37.90	275.00	49.90	493.00	61.90	488.00	73.90	147.00
38.90	1571.00	50.90	868.00	62.95	1285.00	74.95	112.00
39.90	142.00	51.90	203.00	64.00	369.00	76.00	71.00
40.95	234.00	52.90	275.00	64.95	2405.00	77.00	814.00
42.00	27.00	53.95	20.00	66.00	178.00	78.00	110.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.

79.05	329.00	90.05	6514.00	102.00	5.00	116.05	9.00
80.00	31.00	91.05	8236.00	103.05	6.00	118.00	9999.00
80.95	16.00	92.00	740.00	104.00	8.00	119.00	2699.00
81.90	7.00	93.05	60.00	105.05	174.00	120.05	220.00
83.00	6.00	94.00	6.00	106.05	20.00	121.05	72.00
83.95	21.00	95.05	5.00	107.05	88.00	122.05	23.00
84.95	69.00	96.10	1.00	108.05	17.00	122.95	1.00
85.95	116.00	97.00	6.00	109.05	4.00	123.10	4.00
86.95	85.00	98.00	5.00	111.00	1.00	125.05	1.00
88.05	34.00	99.05	1.00	113.05	1.00	125.80	1.00
89.00	1763.00	101.00	4.00	115.10	6.00	129.10	3.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
131.95	4.00	149.05	4.00				
133.05	40.00	150.05	20.00				
134.05	8.00	151.05	0.00				
135.05	297.00	153.05	1.00				
136.05	8734.00	168.95	1.00				
137.05	773.00	181.00	3.00				
138.05	73.00	207.05	1.00				
139.10	6.00	218.95	1.00				
140.95	1.00						
144.95	1.00						
147.05	1.00						

#53: 4-METHYLBENZOIC ACID
Modified: scaled

Entry Number 53 from C:\DATABASE\hjf.l
CAS 000099-94-5
Melting Point -300
Boiling Point -300
Retention Index 75.989
Mol Formula C8H8O2
Mol Weight 136.051
Miscellaneous Information
Aldrich: p-toluic acid

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	32.00	42.00	18.00	51.95	127.00	65.00	1846.00
27.00	160.00	44.90	323.00	52.90	177.00	65.95	123.00
28.90	10.00	45.80	23.00	53.95	39.00	66.95	27.00
33.90	1.00	46.65	0.00	54.95	43.00	67.90	12.00
34.80	2.00	46.85	0.00	56.00	7.00	68.90	2.00
35.90	7.00	47.80	2.00	57.00	7.00	69.95	2.00
36.95	75.00	47.90	3.00	58.95	274.00	71.05	6.00
37.95	167.00	48.05	1.00	60.90	118.00	71.85	3.00
38.90	1022.00	48.90	35.00	61.90	324.00	72.30	1.00

39.90	94.00	49.90	364.00	62.95	819.00	72.90	30.00
40.95	188.00	50.90	508.00	64.00	214.00	73.95	106.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
74.95	80.00	85.90	80.00	95.95	2.00	107.05	306.00
76.00	51.00	87.00	64.00	97.10	6.00	108.00	70.00
77.00	360.00	88.00	26.00	98.10	2.00	109.00	9.00
78.00	59.00	89.00	742.00	99.10	1.00	110.00	3.00
79.00	107.00	90.05	532.00	99.95	1.00	111.05	2.00
80.05	22.00	91.05	9999.00	100.95	6.00	111.90	0.00
81.05	16.00	92.05	1618.00	102.05	1.00	112.15	1.00
82.00	7.00	93.00	95.00	103.00	6.00	114.00	2.00
83.05	6.00	94.05	6.00	104.10	7.00	114.90	1.00
83.95	16.00	94.65	1.00	105.05	93.00	115.10	2.00
84.95	49.00	95.00	4.00	106.05	13.00	116.00	4.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
117.10	7.00	134.05	15.00	168.95	1.00		
118.00	173.00	135.00	161.00	175.95	1.00		
119.05	5559.00	136.05	7380.00	181.00	1.00		
120.05	499.00	137.05	648.00	218.95	2.00		
121.05	47.00	138.05	61.00				
122.05	13.00	139.10	4.00				
123.00	4.00	146.95	1.00				
129.05	1.00	150.05	10.00				
130.95	1.00	151.00	4.00				
131.95	1.00	153.20	1.00				
133.10	8.00	164.00	1.00				

#54: 1,3-BENZODIOXOL-5-OL
Modified: scaled

Entry Number 54 from C:\DATABASE\hjf.l
CAS 000533-31-3
Melting Point -300
Boiling Point -300
Retention Index 80.659
Mol Formula C7H6O3
Mol Weight 138.032
Miscellaneous Information
Fluka: sesamol

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	301.00	38.90	357.00	54.90	297.00	68.90	1392.00
26.90	239.00	39.90	85.00	55.90	15.00	71.05	10.00
28.90	292.00	40.90	201.00	58.00	0.00	72.00	1.00
29.90	41.00	41.90	197.00	59.90	18.00	72.95	4.00
30.90	25.00	47.90	22.00	60.90	96.00	73.95	5.00
32.80	0.00	48.90	102.00	61.90	244.00	74.90	1.00

33.90	95.00	49.90	641.00	62.90	151.00	75.95	2.00
35.15	0.00	50.90	1105.00	64.00	38.00	76.90	53.00
35.85	18.00	51.95	2228.00	65.00	158.00	78.00	25.00
36.90	138.00	52.90	1470.00	65.95	69.00	79.00	521.00
37.90	219.00	53.90	358.00	67.00	39.00	80.05	1303.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
81.05	563.00	97.05	29.00	115.00	0.00	134.00	0.00
82.05	278.00	98.05	1.00	117.05	0.00	135.10	0.00
83.05	17.00	99.05	1.00	120.05	5.00	137.05	8067.00
84.00	27.00	103.00	0.00	121.05	17.00	138.05	9999.00
86.90	0.00	105.00	0.00	122.05	2.00	139.05	805.00
89.95	3.00	107.00	355.00	123.05	7.00	140.05	91.00
92.05	63.00	108.05	207.00	124.05	1.00	141.05	5.00
93.05	33.00	109.05	152.00	125.10	0.00	142.05	1.00
94.05	4.00	110.05	29.00	132.05	0.00	145.05	0.00
95.05	35.00	111.05	4.00	132.40	0.00	147.05	0.00
96.05	43.00	112.10	1.00	133.05	2.00	149.05	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
152.05	1.00	196.20	0.00				
154.30	0.00	197.20	0.00				
155.20	0.00	220.05	0.00				
159.10	1.00	224.25	0.00				
160.05	1.00	225.20	0.00				
161.05	2.00						
161.95	0.00						
163.05	0.00						
167.05	0.00						
175.20	0.00						
181.05	0.00						

#55: 4,6-DINITRO-O-CRESOL
Modified: scaled

Entry Number 55 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 87.079
Mol Formula C7H6N2O5
Mol Weight 198.027

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	82.00	41.95	68.00	54.90	219.00	68.05	232.00
26.90	492.00	43.05	481.00	56.05	70.00	68.90	253.00
28.90	108.00	45.90	24.00	59.05	0.00	69.90	51.00
29.90	1312.00	46.90	4.00	59.95	11.00	72.05	6.00
34.90	0.00	47.95	12.00	60.90	113.00	72.90	61.00

35.90	5.00	48.90	66.00	61.90	311.00	73.90	406.00
36.90	143.00	49.90	1177.00	62.90	534.00	75.00	328.00
37.90	287.00	50.90	2959.00	64.05	364.00	76.05	587.00
38.90	1447.00	52.00	1369.00	65.05	950.00	77.05	1447.00
39.90	249.00	52.90	2301.00	66.05	765.00	78.05	641.00
40.90	113.00	53.90	201.00	66.90	1322.00	79.05	389.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
80.05	157.00	91.05	120.00	104.05	306.00	118.05	19.00
81.05	74.00	92.05	139.00	105.05	3360.00	119.05	49.00
82.05	65.00	93.05	1138.00	106.05	1742.00	121.05	2793.00
83.00	45.00	94.05	299.00	107.05	506.00	122.05	359.00
84.05	9.00	95.05	55.00	108.05	51.00	123.05	65.00
85.05	9.00	96.05	85.00	109.05	14.00	124.05	7.00
86.00	44.00	97.05	9.00	110.05	50.00	126.05	0.00
87.05	50.00	98.05	1.00	111.05	5.00	128.05	0.00
88.05	28.00	101.00	15.00	112.05	1.00	129.05	1.00
89.05	25.00	102.05	7.00	116.05	1.00	130.05	1.00
90.00	93.00	103.05	32.00	117.00	23.00	132.05	2.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
133.05	7.00	146.05	1.00	157.05	2.00	172.10	1.00
134.05	355.00	147.05	1.00	158.15	1.00	176.05	1.00
135.05	12.00	148.05	3.00	159.05	1.00	177.10	1.00
136.05	51.00	149.05	8.00	161.05	0.00	178.05	6.00
137.05	5.00	150.05	40.00	162.05	0.00	179.05	6.00
138.05	16.00	151.05	157.00	165.05	45.00	180.05	286.00
139.05	4.00	152.05	849.00	166.05	12.00	181.05	168.00
140.10	1.00	153.05	71.00	168.05	1883.00	182.05	237.00
143.05	1.00	154.05	8.00	169.05	156.00	183.05	24.00
144.20	0.00	155.10	1.00	170.05	22.00	184.05	5.00
145.05	1.00	156.05	1.00	171.05	2.00	185.05	2.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
191.05	2.00	203.05	0.00	225.25	1.00		
192.10	5.00	205.10	0.00	247.20	2.00		
193.00	1.00	207.05	1.00				
194.05	2.00	208.95	1.00				
195.00	2.00	209.20	1.00				
196.05	30.00	210.05	1.00				
198.05	9999.00	211.20	0.00				
199.05	937.00	212.20	0.00				
200.05	143.00	218.05	0.00				
201.05	10.00	219.95	1.00				
202.05	1.00	224.15	2.00				

#56: 2,3-BENZOFURAN
Modified: scaled

Entry Number 56 from C:\DATABASE\hjf.l

CAS 000271-89-6
Melting Point -300
Boiling Point -300
Retention Index 45.659
Mol Formula C8H6O
Mol Weight 118.042

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	44.00	43.05	138.00	56.05	1.00	67.90	4.00
26.90	52.00	44.90	337.00	56.40	0.00	69.65	0.00
28.90	47.00	46.65	0.00	56.80	1.00	71.95	3.00
34.75	0.00	47.90	8.00	58.95	519.00	72.90	24.00
35.05	0.00	48.90	58.00	60.90	229.00	73.90	80.00
35.90	13.00	49.90	261.00	61.90	626.00	74.90	54.00
36.90	151.00	50.90	293.00	62.90	1562.00	76.00	8.00
37.90	292.00	51.90	22.00	64.00	425.00	76.90	9.00
38.90	600.00	52.90	56.00	64.90	30.00	78.05	1.00
39.90	90.00	53.90	4.00	65.90	14.00	78.95	8.00
40.90	7.00	54.90	10.00	66.90	3.00	80.00	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
83.95	22.00	95.95	1.00	119.05	926.00	153.10	1.00
84.90	78.00	96.95	2.00	120.05	57.00	155.05	0.00
85.95	146.00	98.00	5.00	121.05	3.00	165.05	0.00
86.95	136.00	98.95	1.00	125.90	0.00	176.00	0.00
88.05	17.00	100.95	0.00	126.80	0.00	179.10	1.00
89.05	3477.00	101.80	0.00	127.10	0.00	181.00	0.00
90.05	3546.00	103.00	1.00	128.05	1.00	207.05	1.00
91.05	261.00	104.95	1.00	141.20	0.00		
92.00	22.00	115.05	1.00	150.00	0.00		
92.95	1.00	116.05	8.00	151.00	1.00		
94.05	0.00	118.05	9999.00	152.05	3.00		

#57: 2,6-DIMETHYLPHENOL
Modified: scaled

Entry Number 57 from C:\DATABASE\hjf.l
CAS 000576-26-1
Melting Point -300
Boiling Point -300
Retention Index 60.28
Mol Formula C8H10O
Mol Weight 122.072

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	63.00	39.90	145.00	51.95	317.00	62.90	380.00
26.90	528.00	40.90	342.00	52.95	581.00	64.00	92.00
28.90	55.00	41.95	30.00	53.90	67.00	65.00	716.00

29.90	1.00	42.95	372.00	54.90	145.00	66.00	154.00
32.90	2.00	44.90	131.00	56.00	6.00	67.05	94.00
33.60	0.00	45.90	97.00	56.90	4.00	67.95	16.00
34.85	0.00	46.85	14.00	58.00	1.00	70.00	1.00
35.90	2.00	47.85	4.00	59.00	66.00	71.00	0.00
36.90	57.00	48.95	28.00	59.95	486.00	71.95	1.00
37.90	160.00	49.90	316.00	60.90	177.00	72.95	14.00
38.90	1022.00	50.90	864.00	61.90	155.00	73.90	77.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
74.95	63.00	85.95	30.00	96.95	3.00	110.05	2.00
76.00	83.00	86.95	24.00	97.95	8.00	114.85	0.00
77.05	2576.00	88.00	5.00	98.95	3.00	115.05	0.00
78.05	1360.00	89.00	110.00	101.05	13.00	116.15	0.00
79.05	1880.00	90.05	11.00	102.05	126.00	116.80	0.00
80.05	175.00	91.05	1881.00	103.05	1120.00	117.05	1.00
81.00	52.00	92.05	225.00	104.05	751.00	118.05	1.00
82.00	29.00	93.05	467.00	105.05	369.00	119.00	44.00
83.05	4.00	94.05	351.00	107.05	8913.00	121.05	3310.00
83.90	4.00	95.00	46.00	108.05	702.00	122.05	9999.00
84.95	16.00	96.05	9.00	109.05	44.00	123.05	873.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
124.05	56.00						
125.05	3.00						
132.65	0.00						
135.00	1.00						
147.00	0.00						
158.05	1.00						
165.05	1.00						
166.05	2.00						
169.00	0.00						
181.00	0.00						
184.10	1.00						

#58: 2,5-DIMETHYLRESORCINOL
Modified: scaled

Entry Number 58 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 84.79
Mol Formula C8H10O2
Mol Weight 138.068
Miscellaneous Information
Aldrich: 2,5-dimethyl-1,3-benzenediol

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.

25.90	57.00	39.90	140.00	52.95	622.00	64.05	55.00
26.90	400.00	40.90	457.00	53.90	197.00	65.05	560.00
28.90	114.00	41.90	62.00	54.90	542.00	66.05	201.00
29.95	2.00	42.90	545.00	56.00	32.00	67.00	467.00
32.85	1.00	44.90	35.00	57.05	11.00	68.05	295.00
33.70	0.00	45.90	21.00	58.05	1.00	68.90	387.00
34.65	1.00	46.90	19.00	58.90	48.00	69.90	29.00
35.90	2.00	48.90	21.00	60.00	13.00	71.05	12.00
36.90	36.00	49.90	178.00	60.95	31.00	72.00	2.00
37.90	124.00	50.90	397.00	61.90	59.00	72.90	9.00
38.90	758.00	51.95	161.00	62.90	162.00	74.05	43.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
74.90	37.00	85.95	14.00	97.05	23.00	109.05	763.00
76.00	24.00	86.90	11.00	98.05	12.00	110.05	343.00
77.05	610.00	88.05	3.00	99.05	8.00	111.05	39.00
78.05	107.00	89.05	81.00	101.00	5.00	112.05	5.00
79.05	642.00	90.05	51.00	102.05	6.00	113.15	1.00
80.05	114.00	91.05	1591.00	103.05	17.00	116.95	2.00
81.05	520.00	92.05	386.00	104.05	1.00	118.05	6.00
82.05	115.00	93.05	133.00	105.05	68.00	119.05	329.00
83.05	864.00	94.00	190.00	106.05	8.00	120.05	743.00
84.00	50.00	95.05	1222.00	107.05	200.00	121.05	892.00
85.05	17.00	96.05	140.00	108.05	109.00	123.05	3651.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
124.05	287.00	139.05	910.00	162.05	0.00	208.05	0.00
125.05	27.00	140.05	77.00	165.05	1.00	210.05	1.00
126.05	2.00	141.05	5.00	166.05	0.00	224.30	0.00
127.10	1.00	142.20	0.00	167.05	1.00	225.20	1.00
128.05	0.00	142.95	0.00	175.20	0.00		
129.05	0.00	146.05	0.00	179.20	1.00		
133.00	0.00	147.05	1.00	180.10	1.00		
134.05	1.00	150.05	0.00	182.15	1.00		
135.05	20.00	151.05	1.00	193.00	1.00		
137.05	3882.00	152.05	0.00	194.05	0.00		
138.05	9999.00	155.20	0.00	207.00	0.00		

#59: 3-NITRO-1,2-BENZENEDICARBOXYLIC ACID
Modified: scaled

Entry Number 59 from C:\DATABASE\hjf.l
CAS 000603-11-2
Melting Point -300
Boiling Point -300
Retention Index 92.26
Mol Formula C8H5NO6
Mol Weight 211.012
Miscellaneous Information

Aldrich: 3-nitrophthalic acid

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	49.00	37.90	349.00	49.95	205.00	60.90	276.00
27.00	24.00	38.95	241.00	50.95	116.00	61.95	412.00
27.90	96.00	39.90	31.00	51.95	177.00	63.00	552.00
28.95	25.00	40.95	89.00	52.90	144.00	64.00	334.00
29.90	545.00	42.00	11.00	53.95	25.00	65.00	287.00
30.90	3.00	43.05	27.00	55.00	38.00	66.05	36.00
33.35	4.00	43.90	471.00	57.05	31.00	67.00	16.00
33.65	3.00	45.45	201.00	58.00	4.00	68.05	13.00
35.15	2.00	47.05	2.00	58.30	3.00	68.95	63.00
35.95	55.00	47.95	36.00	59.60	54.00	70.05	9.00
36.90	554.00	48.90	274.00	59.80	59.00	71.05	25.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
72.05	30.00	83.05	9.00	94.05	14.00	105.05	324.00
73.05	451.00	84.05	10.00	95.05	13.00	106.05	38.00
74.00	2819.00	85.10	15.00	96.05	13.00	107.05	71.00
75.00	9999.00	86.00	23.00	97.05	6.00	108.05	21.00
76.00	712.00	87.00	34.00	98.10	5.00	109.05	15.00
77.00	192.00	88.00	41.00	99.10	1.00	110.05	11.00
78.05	54.00	89.05	148.00	100.00	9.00	111.10	4.00
79.00	36.00	90.00	99.00	101.00	20.00	112.05	8.00
80.05	13.00	91.05	1258.00	102.00	27.00	113.10	4.00
81.05	15.00	92.05	123.00	103.05	1401.00	113.95	4.00
82.00	11.00	93.05	51.00	104.00	134.00	115.00	7.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
116.05	10.00	127.10	6.00	138.00	7.00	151.05	64.00
117.05	163.00	128.10	3.00	139.15	3.00	152.05	30.00
118.05	30.00	129.10	6.00	140.10	8.00	153.05	8.00
119.05	535.00	130.10	9.00	141.15	7.00	154.05	6.00
120.05	65.00	131.05	29.00	143.10	2.00	155.15	7.00
121.05	102.00	132.05	1.00	144.10	11.00	155.95	2.00
122.05	15.00	133.00	42.00	145.05	9.00	156.20	2.00
123.05	8.00	134.05	13.00	146.05	5.00	157.15	3.00
124.10	3.00	135.05	42.00	147.05	30.00	159.20	2.00
125.15	2.00	136.05	8.00	149.05	6639.00	161.05	39.00
126.10	1.00	137.05	52.00	150.05	541.00	162.05	24.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
163.05	1115.00	179.05	88.00	207.05	15.00		
164.05	115.00	180.05	11.00	208.05	7.00		
165.05	20.00	181.05	3.00	209.05	3.00		
166.15	3.00	189.10	9.00	219.00	21.00		
167.10	10.00	191.05	18.00	220.10	7.00		
168.20	2.00	192.05	4.00				
169.05	6.00	193.05	72.00				
175.10	11.00	194.00	21.00				
176.05	2.00	195.05	3.00				

177.05	65.00	196.20	2.00
178.05	14.00	204.95	2.00

#60: 3-METHYLBENZOIC ACID
Modified: scaled

Entry Number 60 from C:\DATABASE\hjf.l
CAS 000099-04-7
Melting Point -300
Boiling Point -300
Retention Index 75.23
Mol Formula C8H8O2
Mol Weight 136.051
Miscellaneous Information
Aldrich: m-toluic acid

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	32.00	42.10	22.00	54.05	26.00	64.00	213.00
28.90	25.00	44.90	278.00	55.00	53.00	65.00	1752.00
33.95	2.00	45.90	7.00	56.10	13.00	66.00	117.00
34.60	5.00	46.75	13.00	57.00	31.00	67.00	44.00
35.95	13.00	47.05	4.00	57.65	1.00	67.95	22.00
36.90	78.00	47.85	8.00	57.90	8.00	70.00	7.00
37.90	168.00	48.90	43.00	58.95	214.00	71.00	18.00
38.90	1075.00	49.90	330.00	59.80	24.00	71.80	2.00
39.90	82.00	50.90	512.00	60.90	117.00	72.15	5.00
40.95	190.00	52.00	127.00	61.95	335.00	72.90	38.00
41.95	9.00	53.00	170.00	62.95	804.00	73.95	112.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
75.00	90.00	85.95	84.00	95.05	7.00	106.00	17.00
76.00	58.00	87.05	63.00	95.95	4.00	107.00	195.00
77.00	417.00	88.10	32.00	96.15	3.00	108.05	57.00
78.05	72.00	89.00	766.00	97.00	7.00	109.00	15.00
79.00	176.00	90.00	674.00	99.05	3.00	112.15	2.00
80.05	34.00	91.00	9999.00	99.90	3.00	113.95	1.00
81.00	17.00	92.00	1770.00	101.00	11.00	115.10	8.00
82.00	11.00	93.00	116.00	102.90	7.00	116.05	3.00
83.10	15.00	93.95	7.00	103.30	3.00	117.00	27.00
83.95	20.00	94.10	10.00	104.00	5.00	118.05	343.00
85.00	58.00	94.90	3.00	105.00	103.00	119.05	3603.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
120.05	320.00	144.95	3.00				
121.05	79.00	147.05	15.00				
122.00	30.00	150.00	9.00				
123.05	2.00	169.00	3.00				
131.95	4.00	218.95	2.00				
133.05	16.00						

134.00	17.00
135.05	409.00
136.05	6887.00
137.05	603.00
138.05	68.00

#61: 1-(2,4,6-TRIMETHYLPHENYL)-ETHANONE
Modified: scaled

Entry Number 61 from C:\DATABASE\hjf.l
CAS 001667-01-2
Melting Point -300
Boiling Point -300
Retention Index 70.379
Mol Formula C11H14O
Mol Weight 162.104
Miscellaneous Information
Aldrich: 2',4',6'-trimethylacetophenone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.15	0.00	37.90	33.00	51.90	136.00	64.00	72.00
25.95	11.00	38.90	454.00	53.00	222.00	65.05	410.00
26.90	191.00	39.90	50.00	54.00	13.00	66.00	184.00
28.90	24.00	40.95	540.00	55.00	37.00	66.95	32.00
29.95	0.00	42.00	29.00	56.00	1.00	67.95	2.00
33.80	0.00	42.95	485.00	57.50	109.00	69.80	0.00
34.35	1.00	47.85	0.00	59.30	8.00	70.05	3.00
34.65	0.00	48.05	0.00	59.55	2.00	71.00	11.00
35.05	0.00	48.95	3.00	60.95	12.00	72.50	35.00
35.85	0.00	49.90	121.00	61.90	61.00	73.75	73.00
36.85	8.00	50.90	429.00	62.95	213.00	74.95	63.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
76.00	58.00	86.00	16.00	96.15	0.00	107.00	4.00
77.05	839.00	86.95	23.00	96.95	2.00	108.10	1.00
78.00	306.00	88.00	9.00	98.00	10.00	108.95	1.00
79.05	300.00	89.05	101.00	99.00	5.00	110.05	2.00
80.05	107.00	90.00	5.00	99.95	0.00	111.05	1.00
81.80	0.00	91.05	1772.00	101.00	18.00	112.05	0.00
82.10	1.00	92.05	148.00	102.05	117.00	113.05	5.00
82.90	1.00	93.00	149.00	103.05	483.00	114.00	0.00
83.15	0.00	94.05	11.00	104.05	300.00	115.05	648.00
83.95	1.00	95.00	1.00	105.05	190.00	116.05	158.00
84.95	5.00	95.90	0.00	106.05	17.00	117.05	728.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
118.05	188.00	131.00	41.00	143.05	10.00	164.05	25.00
119.05	5941.00	132.00	24.00	144.05	5.00	165.15	2.00
120.05	573.00	133.05	76.00	145.05	30.00	169.00	0.00

121.05	25.00	134.15	9.00	147.05	9999.00	176.20	0.00
122.05	2.00	134.80	0.00	148.05	1097.00		
125.00	0.00	135.10	1.00	149.05	72.00		
126.05	7.00	137.05	0.00	150.00	3.00		
127.05	33.00	139.05	3.00	159.05	12.00		
128.05	83.00	140.05	1.00	160.05	11.00		
129.05	50.00	141.05	9.00	162.05	2939.00		
130.05	11.00	142.10	3.00	163.05	357.00		

#62: 4'-HYDROXY-3'-METHYLACETOPHENONE
Modified: scaled

Entry Number 62 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 86.95
Mol Formula C9H10O2
Mol Weight 150.068

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	28.00	39.90	40.00	54.90	94.00	67.05	136.00
26.90	216.00	40.90	51.00	56.05	5.00	70.05	0.00
28.90	39.00	41.95	34.00	57.05	2.00	71.05	2.00
29.90	0.00	42.90	748.00	58.55	45.00	72.05	1.00
33.05	0.00	46.95	2.00	60.00	84.00	72.90	15.00
35.05	0.00	47.85	2.00	60.90	65.00	73.95	87.00
35.30	0.00	48.90	19.00	61.90	93.00	75.00	51.00
36.05	1.00	49.90	231.00	62.95	230.00	76.00	61.00
36.85	28.00	50.90	562.00	64.05	48.00	77.05	2105.00
37.90	97.00	51.90	301.00	65.00	97.00	78.00	454.00
38.90	542.00	53.00	466.00	65.95	48.00	79.05	1162.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
80.05	87.00	91.05	159.00	103.05	20.00	114.00	0.00
81.05	18.00	92.05	23.00	104.05	6.00	115.05	5.00
82.05	2.00	93.05	25.00	105.05	119.00	116.05	1.00
83.00	1.00	94.05	8.00	106.05	221.00	117.05	14.00
84.05	2.00	95.05	1.00	107.05	2564.00	118.00	5.00
85.05	9.00	96.05	0.00	108.05	211.00	119.05	13.00
85.95	17.00	97.05	2.00	109.05	15.00	120.05	11.00
87.05	16.00	98.05	3.00	110.10	1.00	121.05	110.00
88.00	7.00	99.05	1.00	111.05	0.00	122.05	11.00
89.05	61.00	101.05	4.00	112.10	0.00	123.05	1.00
90.00	29.00	102.05	8.00	113.05	1.00	124.05	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
125.05	1.00	138.00	5.00	152.05	44.00	165.05	1.00
126.10	1.00	139.15	1.00	153.05	4.00	166.05	1.00

127.15	0.00	141.15	0.00	154.20	0.00	168.20	0.00
128.10	1.00	143.05	0.00	155.20	1.00	169.05	0.00
129.10	1.00	144.80	0.00	158.05	0.00	175.95	0.00
131.00	1.00	145.05	0.00	159.05	0.00	177.05	2.00
132.00	3.00	147.05	11.00	159.95	1.00	178.10	1.00
133.00	23.00	148.05	6.00	161.10	1.00	179.05	0.00
135.05	9999.00	149.15	21.00	162.10	1.00	180.15	0.00
136.05	938.00	150.05	4363.00	163.05	1.00	181.00	1.00
137.05	83.00	151.05	502.00	164.05	0.00	185.05	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
191.00	0.00	228.20	0.00				
193.05	0.00	229.20	0.00				
194.95	1.00	229.95	2.00				
195.20	0.00	231.90	2.00				
196.20	0.00	232.95	0.00				
197.05	0.00	233.95	0.00				
206.20	1.00						
207.00	0.00						
209.10	1.00						
211.15	1.00						
224.05	0.00						

#63: 3,4-DIMETHYLPHENOL
Modified: scaled

Entry Number 63 from C:\DATABASE\hjf.l
CAS 000095-65-8
Melting Point -300
Boiling Point -300
Retention Index 69.65
Mol Formula C8H10O
Mol Weight 122.072

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.85	58.00	37.90	153.00	49.90	295.00	60.95	161.00
26.90	473.00	38.90	897.00	50.90	718.00	61.90	118.00
28.90	76.00	39.90	136.00	51.95	284.00	62.90	270.00
29.95	2.00	41.00	307.00	52.95	530.00	64.00	70.00
30.90	10.00	41.90	40.00	53.90	54.00	65.05	543.00
32.85	2.00	43.00	161.00	54.90	234.00	66.00	152.00
33.00	0.00	44.90	61.00	56.00	9.00	67.05	136.00
34.85	1.00	45.90	73.00	57.00	3.00	68.00	26.00
35.30	0.00	46.85	14.00	58.00	1.00	68.95	4.00
35.95	2.00	48.05	2.00	59.00	100.00	69.95	2.00
36.90	50.00	48.90	34.00	60.00	328.00	71.05	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
71.95	1.00	83.05	5.00	94.05	181.00	107.05	9999.00

72.95	14.00	83.95	3.00	95.05	42.00	108.05	796.00
73.95	78.00	84.90	11.00	96.00	6.00	109.05	51.00
74.90	61.00	85.90	21.00	96.95	3.00	110.05	3.00
76.00	55.00	87.00	17.00	98.05	10.00	114.95	0.00
77.05	2184.00	88.05	4.00	99.00	3.00	117.05	1.00
78.05	443.00	89.05	76.00	101.00	14.00	118.05	11.00
79.05	907.00	90.00	7.00	102.05	53.00	119.00	80.00
80.00	78.00	91.05	1366.00	103.05	322.00	120.05	137.00
81.00	85.00	92.05	153.00	104.05	133.00	121.05	4041.00
82.05	24.00	93.05	259.00	105.05	176.00	122.05	8065.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
123.05	702.00	144.95	0.00				
124.05	48.00	158.10	1.00				
125.05	3.00	159.05	0.00				
125.90	0.00	165.10	1.00				
128.05	0.00	166.05	2.00				
129.15	0.00	167.05	0.00				
130.05	0.00	169.00	0.00				
133.20	0.00	175.95	0.00				
135.10	1.00	181.05	1.00				
142.95	0.00	184.10	1.00				
143.20	0.00						

#64: 1-(4-HYDROXYPHENYL)-ETHANONE
Modified: scaled

Entry Number 64 from C:\DATABASE\hjf.l
CAS 000099-93-4
Melting Point -300
Boiling Point -300
Retention Index 86.29
Mol Formula C8H8O2
Mol Weight 136.051
Miscellaneous Information
Aldrich: 4'-hydroxyacetophenone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	33.00	38.90	1248.00	52.90	354.00	64.00	307.00
26.90	109.00	39.90	69.00	54.00	99.00	65.05	2277.00
28.90	43.00	40.90	12.00	54.90	68.00	66.05	251.00
29.95	1.00	41.90	60.00	56.00	3.00	67.00	33.00
30.90	9.00	43.05	804.00	57.05	3.00	68.00	9.00
34.05	0.00	46.00	82.00	58.30	1.00	70.00	1.00
34.30	1.00	47.90	2.00	58.90	2.00	71.05	4.00
34.65	0.00	48.90	32.00	59.10	4.00	72.00	2.00
35.95	6.00	49.90	208.00	60.50	147.00	72.95	24.00
36.90	79.00	50.90	243.00	61.90	206.00	73.90	107.00

37.90	221.00	52.00	72.00	62.95	468.00	75.00	75.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
76.05	34.00	87.00	8.00	98.05	4.00	109.05	1.00
77.05	268.00	88.05	2.00	99.10	1.00	110.10	1.00
78.05	53.00	89.05	21.00	100.95	2.00	111.10	1.00
79.00	80.00	90.05	10.00	101.95	1.00	112.05	1.00
80.00	7.00	91.05	29.00	102.30	1.00	113.10	2.00
81.05	8.00	92.05	194.00	103.05	1.00	114.00	0.00
82.05	1.00	93.05	3719.00	104.00	4.00	116.05	0.00
83.05	0.00	94.05	309.00	105.05	11.00	117.05	2.00
84.05	3.00	95.05	19.00	106.10	1.00	118.05	7.00
85.05	10.00	96.05	1.00	107.05	92.00	119.00	17.00
86.00	12.00	97.05	2.00	108.05	8.00	121.05	9999.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.05	793.00	137.05	345.00	161.20	1.00	209.05	1.00
123.00	70.00	138.00	29.00	163.05	0.00	218.95	0.00
124.05	6.00	139.05	3.00	165.05	3.00		
125.10	1.00	141.05	2.00	167.20	1.00		
126.05	0.00	145.05	0.00	169.00	0.00		
127.10	1.00	147.05	1.00	180.10	1.00		
128.05	0.00	149.05	0.00	181.05	1.00		
129.15	1.00	150.00	1.00	191.05	0.00		
131.90	2.00	151.00	1.00	193.05	1.00		
133.05	1.00	152.05	1.00	207.05	0.00		
136.05	3671.00	155.15	1.00	208.00	1.00		

#65: 4-METHYLBENZENEMETHANOL
Modified: scaled

Entry Number 65 from C:\DATABASE\hjf.l
CAS 000589-18-4
Melting Point -300
Boiling Point -300
Retention Index 61.689
Mol Formula C8H10O
Mol Weight 122.072
Miscellaneous Information
Aldrich: 4-methylbenzyl alcohol

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	60.00	37.90	230.00	50.90	1381.00	60.80	108.00
26.95	534.00	38.90	1619.00	51.95	377.00	61.90	344.00
28.90	263.00	39.95	180.00	53.00	429.00	62.95	898.00
29.90	17.00	40.95	428.00	53.90	31.00	64.00	208.00
30.90	201.00	42.00	31.00	54.95	85.00	65.05	2182.00
32.95	3.00	44.90	50.00	55.95	5.00	66.00	209.00
33.65	0.00	45.90	64.00	57.00	6.00	67.05	43.00

33.90	1.00	46.95	21.00	57.80	2.00	67.95	15.00
34.55	2.00	47.90	3.00	58.05	1.00	70.00	1.00
35.95	5.00	48.95	49.00	59.05	89.00	70.80	0.00
36.85	85.00	49.90	579.00	60.00	731.00	71.10	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
71.95	3.00	83.05	2.00	94.05	370.00	107.05	9999.00
72.90	31.00	83.95	7.00	95.00	19.00	108.05	763.00
73.95	172.00	84.95	39.00	95.95	1.00	109.05	50.00
74.95	127.00	85.95	80.00	97.00	6.00	110.05	4.00
76.00	141.00	87.00	66.00	98.00	19.00	115.00	1.00
77.05	5377.00	88.00	17.00	99.00	6.00	115.95	1.00
78.05	1168.00	89.05	543.00	101.05	17.00	116.10	1.00
79.05	6708.00	90.00	180.00	102.05	122.00	117.05	4.00
80.05	449.00	91.05	6287.00	103.05	806.00	119.05	678.00
81.00	35.00	92.05	637.00	104.05	1329.00	120.05	407.00
82.05	7.00	93.05	4617.00	105.05	1560.00	121.05	1643.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.05	9930.00						
123.05	848.00						
124.05	55.00						
125.05	4.00						
128.10	2.00						
129.10	1.00						
131.95	1.00						
142.05	1.00						
154.10	2.00						
169.00	3.00						
181.05	0.00						

#66: 1-(4-METHOXYPHENYL)-ETHANONE
Modified: scaled

Entry Number 66 from C:\DATABASE\hjf.l
CAS 000100-06-1
Melting Point -300
Boiling Point -300
Retention Index 77.409
Mol Formula C9H10O2
Mol Weight 150.068
Miscellaneous Information
Aldrich: 4'-methoxyacetophenone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	18.00	38.90	211.00	52.00	91.00	65.00	167.00
26.90	64.00	39.90	11.00	52.95	119.00	65.95	50.00
28.90	23.00	40.95	15.00	53.90	8.00	67.05	19.00
29.95	3.00	42.00	32.00	54.95	10.00	72.00	0.00

31.00	4.00	42.95	716.00	58.30	0.00	72.95	21.00
32.80	0.00	46.80	0.00	59.00	2.00	73.95	135.00
33.05	0.00	47.05	0.00	60.00	7.00	75.00	100.00
33.95	0.00	47.85	1.00	60.90	85.00	76.05	225.00
35.90	1.00	48.90	18.00	61.95	140.00	77.05	2612.00
36.90	39.00	49.90	326.00	63.00	593.00	78.05	306.00
37.90	176.00	50.90	305.00	64.05	779.00	79.05	191.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
80.05	14.00	94.00	10.00	109.05	10.00	124.00	0.00
81.05	2.00	95.05	2.00	110.05	1.00	132.00	1.00
83.30	0.00	96.10	0.00	111.40	0.00	133.05	22.00
85.95	9.00	98.00	3.00	116.05	1.00	135.05	9999.00
87.00	8.00	101.00	3.00	117.00	2.00	136.05	869.00
88.00	3.00	102.05	3.00	118.00	4.00	137.05	69.00
89.05	42.00	103.00	7.00	119.05	55.00	138.05	5.00
90.00	13.00	104.05	49.00	120.05	47.00	139.05	0.00
91.05	121.00	105.00	28.00	121.05	61.00	147.80	0.00
92.05	1296.00	107.05	1968.00	122.05	7.00	150.05	3597.00
93.05	103.00	108.05	158.00	123.05	2.00	151.05	352.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
152.05	29.00						
153.15	2.00						
180.95	0.00						
219.95	0.00						

#67: 1-(3-NITROPHENYL)-ETHANONE
Modified: scaled

Entry Number 67 from C:\DATABASE\hjf.l
CAS 000121-89-1
Melting Point -300
Boiling Point -300
Retention Index 83.56
Mol Formula C8H7NO3
Mol Weight 165.042
Miscellaneous Information
Aldrich: 3'-nitroacetophenone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	14.00	39.90	17.00	54.00	4.00	66.95	3.00
26.95	41.00	41.00	23.00	54.95	2.00	68.05	1.00
28.90	6.00	42.00	86.00	58.95	1.00	70.15	0.00
29.90	73.00	42.90	2488.00	59.30	1.00	72.00	2.00
33.10	1.00	45.90	2.00	59.90	5.00	72.95	45.00
33.80	0.00	48.00	2.00	60.90	46.00	73.95	322.00
34.95	0.00	49.00	34.00	61.90	108.00	75.00	547.00
35.95	2.00	49.90	899.00	63.00	239.00	76.05	1676.00

36.90	52.00	50.90	420.00	64.05	181.00	77.05	503.00
37.90	100.00	51.90	41.00	65.05	324.00	78.05	37.00
38.90	181.00	52.90	32.00	66.00	23.00	79.05	4.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
80.00	1.00	92.05	474.00	107.05	1.00	121.05	5.00
81.30	0.00	93.05	32.00	108.05	1.00	122.05	207.00
82.55	0.00	94.00	2.00	108.80	0.00	123.05	21.00
83.95	1.00	97.05	1.00	111.40	0.00	124.05	2.00
85.05	9.00	98.05	8.00	112.10	0.00	125.00	0.00
86.00	19.00	99.05	2.00	115.00	1.00	130.05	1.00
87.00	19.00	101.00	9.00	115.95	0.00	132.05	0.00
88.00	11.00	102.05	8.00	117.05	2.00	133.05	1.00
89.05	162.00	104.05	3062.00	118.05	15.00	134.05	20.00
90.05	77.00	105.05	228.00	119.05	86.00	135.05	27.00
91.05	473.00	106.05	15.00	120.05	56.00	136.05	9.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
137.05	1.00	165.05	1643.00				
137.95	0.00	166.05	156.00				
146.00	1.00	167.05	16.00				
147.00	1.00	168.05	2.00				
150.05	9999.00	181.05	0.00				
151.05	853.00						
152.05	93.00						
153.05	6.00						
154.10	1.00						
161.05	0.00						
163.05	0.00						

#68: 2-METHYLFURAN
Modified: scaled

Entry Number 68 from C:\DATABASE\hjf.l
CAS 000534-22-5
Melting Point -300
Boiling Point -300
Retention Index 15.689
Mol Formula C5H6O
Mol Weight 82.042

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	369.00	40.00	134.00	53.00	5428.00	65.95	14.00
26.90	1552.00	40.90	288.00	54.05	1010.00	66.95	8.00
27.90	581.00	41.90	169.00	54.90	259.00	68.00	1.00
28.90	312.00	42.90	649.00	55.95	65.00	75.40	1.00
29.95	4.00	44.90	1.00	57.00	4.00	75.80	1.00
30.90	14.00	45.85	2.00	60.00	11.00	76.90	11.00
32.95	0.00	47.95	18.00	60.90	32.00	77.95	3.00

35.90	39.00	48.90	136.00	61.95	30.00	78.95	30.00
36.85	244.00	49.90	853.00	63.00	60.00	80.05	35.00
37.90	424.00	50.90	1077.00	64.00	27.00	81.05	5887.00
38.90	3150.00	51.90	531.00	65.00	10.00	82.05	9999.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
83.00	567.00						
83.90	4.00						
84.95	0.00						
91.00	3.00						
131.90	0.00						

#69: FURAN
Modified: scaled

Entry Number 69 from C:\DATABASE\hjf.l
CAS 000110-00-9
Melting Point -300
Boiling Point -300
Retention Index 11.21
Mol Formula C4H4O
Mol Weight 68.025

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	180.00	38.90	8555.00	52.90	24.00	68.95	460.00
26.90	45.00	39.90	1199.00	53.95	2.00	70.00	31.00
27.90	57.00	40.90	130.00	54.90	1.00	71.00	2.00
28.90	941.00	41.90	744.00	55.15	0.00	75.90	0.00
29.90	12.00	42.95	18.00	56.05	0.00	77.05	5.00
30.90	0.00	46.90	0.00	59.90	0.00	78.00	2.00
32.95	12.00	47.90	18.00	62.90	1.00	79.00	1.00
33.85	218.00	48.90	64.00	63.90	2.00	80.90	0.00
35.85	125.00	49.85	77.00	64.95	6.00	84.05	0.00
36.90	818.00	50.85	21.00	66.00	31.00	104.90	0.00
37.90	1397.00	51.90	10.00	68.00	9999.00	105.15	0.00

#70: 2-METHYL-2-PROPENOIC ACID
Modified: scaled

Entry Number 70 from C:\DATABASE\hjf.l
CAS 000079-41-4
Melting Point -300
Boiling Point -300
Retention Index 38.159
Mol Formula C4H6O2
Mol Weight 86.037
Miscellaneous Information

Aldrich: methacrylic acid

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	232.00	34.65	2.00	47.95	6.00	59.00	26.00
26.95	531.00	35.90	75.00	48.90	12.00	59.90	75.00
27.90	46.00	36.90	547.00	49.95	19.00	60.80	1.00
28.90	316.00	37.90	983.00	50.90	11.00	61.05	4.00
29.90	65.00	38.90	5889.00	51.95	17.00	62.05	3.00
30.95	84.00	39.95	1747.00	52.90	222.00	62.95	0.00
32.95	7.00	40.95	8486.00	53.95	24.00	63.80	3.00
33.65	2.00	41.95	776.00	54.95	105.00	63.90	2.00
33.80	2.00	44.90	1155.00	56.00	17.00	64.95	5.00
34.00	2.00	45.90	41.00	57.00	434.00	65.90	13.00
34.30	2.00	46.90	38.00	58.05	624.00	67.00	21.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
67.95	1217.00	78.00	5.00	90.05	1.00	101.00	5.00
68.90	1614.00	79.05	5.00	90.30	2.00	104.05	1.00
70.00	83.00	79.90	3.00	91.00	4.00	105.00	12.00
70.90	272.00	80.95	4.00	92.10	6.00	107.05	1.00
71.95	10.00	82.00	1.00	92.95	5.00	118.95	5.00
72.95	10.00	83.95	2.00	93.95	1.00	122.05	4.00
73.95	3.00	85.05	562.00	95.05	0.00	125.90	1.00
74.90	1.00	86.05	9999.00	97.00	3.00	129.00	3.00
75.80	2.00	87.00	480.00	97.30	2.00	132.00	1.00
76.05	1.00	87.95	59.00	98.15	1.00	136.00	7.00
76.95	8.00	89.05	2.00	99.90	1.00	136.20	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
145.05	2.00						

#71: 2-NITROSOTOLUENE
Modified: scaled

Entry Number 71 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 47.63
Mol Formula C7H7NO
Mol Weight 121.052

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	90.00	39.90	173.00	56.05	1.00	68.00	13.00
26.90	213.00	41.00	517.00	57.10	1.00	70.05	1.00
28.90	17.00	42.05	32.00	58.55	2.00	71.90	7.00
29.90	158.00	47.90	10.00	60.05	13.00	72.90	42.00
30.90	10.00	48.90	81.00	60.90	188.00	73.95	188.00
32.85	1.00	49.85	703.00	61.90	524.00	74.95	178.00

34.40	1.00	50.90	1104.00	62.95	1650.00	76.05	185.00
35.90	13.00	51.90	357.00	64.05	499.00	77.05	258.00
36.90	175.00	52.85	91.00	65.05	8815.00	78.00	140.00
37.90	385.00	53.80	28.00	66.00	1165.00	79.05	128.00
38.90	2335.00	55.00	9.00	67.05	147.00	80.05	25.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
81.05	10.00	92.05	1225.00	104.05	142.00	120.05	816.00
82.05	2.00	93.05	4410.00	105.05	20.00	121.05	3413.00
83.05	1.00	94.05	357.00	106.05	511.00	122.05	294.00
83.90	15.00	95.05	13.00	107.05	399.00	123.05	39.00
84.90	55.00	96.05	1.00	108.05	33.00	124.05	3.00
86.00	110.00	97.90	3.00	109.10	2.00	128.05	1.00
87.05	85.00	99.05	14.00	115.15	2.00	129.05	2.00
88.05	30.00	99.95	4.00	116.05	6.00	130.05	2.00
89.05	999.00	101.05	2.00	117.05	13.00	132.05	2.00
90.05	279.00	102.05	16.00	118.05	14.00	133.05	4.00
91.05	9999.00	103.00	19.00	119.05	6.00	135.05	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
143.05	1.00						
144.20	1.00						
164.00	0.00						
167.00	2.00						
168.05	4.00						
169.00	1.00						
218.95	1.00						

#72: 2,4-DIMETHYLBENZALDEHYDE
Modified: scaled

Entry Number 72 from C:\DATABASE\hjf.l
CAS 015764-16-6
Melting Point -300
Boiling Point -300
Retention Index 62.549
Mol Formula C9H10O
Mol Weight 134.073

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	30.00	40.90	117.00	57.35	29.00	70.80	0.00
26.90	461.00	42.00	7.00	58.95	18.00	71.95	2.00
28.90	102.00	48.00	1.00	59.90	6.00	72.90	23.00
29.95	2.00	49.00	27.00	60.90	66.00	73.95	140.00
33.85	1.00	49.90	332.00	61.90	206.00	75.00	118.00
35.40	0.00	50.90	969.00	62.90	545.00	76.05	122.00
35.95	1.00	51.95	249.00	64.00	115.00	77.05	2021.00
36.90	48.00	53.00	338.00	65.05	505.00	78.05	635.00
37.90	139.00	53.95	29.00	66.00	199.00	79.05	1842.00

38.90	943.00	54.95	27.00	66.95	126.00	80.05	120.00
39.90	90.00	56.05	2.00	70.40	0.00	81.00	5.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
82.15	0.00	93.00	3.00	105.05	6451.00	117.05	6.00
83.05	0.00	94.00	1.00	106.05	676.00	118.05	14.00
84.00	3.00	95.05	0.00	107.05	42.00	119.05	71.00
85.00	19.00	96.00	1.00	108.05	2.00	120.00	6.00
86.00	45.00	97.00	5.00	108.95	2.00	121.00	1.00
87.00	42.00	98.00	30.00	110.00	2.00	127.90	0.00
88.00	13.00	99.05	8.00	111.00	1.00	128.15	1.00
89.05	211.00	101.00	23.00	113.00	3.00	129.05	2.00
90.00	67.00	102.05	177.00	114.00	2.00	130.10	2.00
91.05	1158.00	103.05	1310.00	115.05	39.00	131.00	13.00
92.05	85.00	104.05	359.00	116.05	7.00	133.05	9999.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
134.05	8641.00	183.15	1.00				
135.05	841.00	211.15	3.00				
136.05	50.00	212.20	0.00				
137.10	3.00	239.20	2.00				
142.10	1.00						
143.05	0.00						
152.05	0.00						
155.05	0.00						
167.05	0.00						
168.10	2.00						
180.95	1.00						

#73: 1,3-ISOBENZOFURANDIONE
Modified: scaled

Entry Number 73 from C:\DATABASE\hjf.l
CAS 000085-44-9
Melting Point -300
Boiling Point -300
Retention Index 79.28
Mol Formula C8H4O3
Mol Weight 148.015
Miscellaneous Information
Aldrich: phthalic anhydride

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	79.00	40.95	3.00	58.05	0.00	72.00	40.00
27.00	39.00	42.05	4.00	59.90	55.00	72.90	419.00
28.90	13.00	47.90	56.00	60.90	171.00	73.90	1647.00
30.90	28.00	48.90	475.00	61.95	101.00	75.00	1133.00
33.65	0.00	49.90	4703.00	62.95	110.00	76.05	8508.00
34.15	0.00	50.90	295.00	64.00	34.00	77.05	695.00

36.00	87.00	51.90	620.00	64.95	22.00	78.00	31.00
36.95	840.00	52.90	144.00	65.95	44.00	79.00	1.00
37.90	1255.00	53.90	7.00	67.90	2.00	79.95	0.00
38.90	129.00	56.05	0.00	70.00	1.00	81.00	1.00
39.90	6.00	56.30	0.00	70.80	0.00	83.05	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
83.30	0.00	101.00	10.00	134.95	0.00	195.05	1.00
83.95	11.00	102.05	4.00	142.00	2.00	196.05	15.00
85.00	14.00	104.05	9999.00	148.05	3446.00	197.05	3.00
85.90	8.00	105.05	756.00	149.05	300.00	208.10	3.00
87.00	2.00	106.05	46.00	150.00	30.00	223.05	4.00
87.90	0.00	107.05	2.00	151.05	3.00	224.05	1.00
88.95	2.00	113.05	0.00	152.10	2.00		
90.00	3.00	119.00	1.00	168.05	7.00		
91.00	4.00	120.05	1.00	169.00	1.00		
92.00	14.00	121.05	1.00	170.05	11.00		
93.00	1.00	132.05	2.00	171.15	1.00		

#74: PHENOL
Modified: scaled

Entry Number 74 from C:\DATABASE\hjf.l
CAS 000108-95-2
Melting Point -300
Boiling Point -300
Retention Index 56
Mol Formula C6H6O
Mol Weight 94.042

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	80.00	37.90	452.00	52.90	247.00	61.90	213.00
26.90	192.00	38.90	1540.00	53.90	38.00	62.95	459.00
28.90	81.00	39.95	871.00	54.90	651.00	64.00	177.00
29.90	1.00	40.90	57.00	55.95	22.00	65.05	1954.00
30.90	78.00	41.90	64.00	57.00	2.00	66.00	2734.00
31.90	30.00	45.90	46.00	57.65	0.00	67.05	183.00
33.95	3.00	46.95	402.00	57.90	0.00	68.00	86.00
34.80	0.00	48.90	67.00	58.15	0.00	69.95	1.00
35.05	0.00	49.90	382.00	59.00	0.00	71.15	0.00
35.90	25.00	50.90	368.00	59.95	29.00	72.00	5.00
36.90	220.00	52.00	68.00	60.90	133.00	72.90	46.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
73.90	146.00	88.90	2.00	114.90	0.00		
74.95	65.00	89.95	4.00	115.15	0.00		
76.05	63.00	91.00	6.00	131.95	1.00		
77.00	71.00	92.05	23.00	141.05	0.00		
78.05	7.00	93.00	200.00	150.00	0.00		

78.95	69.00	94.05	9999.00	219.95	0.00
80.00	5.00	95.05	704.00		
81.00	1.00	96.00	40.00		
84.10	1.00	97.10	2.00		
85.90	0.00	103.10	0.00		
87.65	0.00	105.05	1.00		

#75: 3-METHYL-2-NITROBENZYL ALCOHOL
Modified: scaled

Entry Number 75 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 83.76
Mol Formula C8H9NO3
Mol Weight 167.057

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	87.00	39.90	347.00	52.00	886.00	62.90	1738.00
26.90	834.00	40.95	1218.00	52.90	1274.00	64.05	750.00
28.90	481.00	41.95	133.00	54.00	197.00	65.05	6815.00
29.90	398.00	42.90	1700.00	55.00	319.00	66.05	2213.00
30.90	391.00	44.90	7.00	55.95	16.00	67.05	542.00
32.90	3.00	45.90	20.00	56.90	16.00	68.05	135.00
34.00	2.00	46.90	85.00	58.00	2.00	68.95	99.00
36.00	2.00	47.85	8.00	58.95	45.00	70.00	25.00
36.90	118.00	48.90	51.00	59.90	43.00	71.00	0.00
37.90	377.00	49.90	761.00	60.90	153.00	71.95	2.00
38.90	2807.00	50.90	2206.00	61.90	522.00	72.95	36.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
73.95	255.00	84.95	40.00	96.05	19.00	107.05	584.00
74.95	320.00	86.00	110.00	97.00	9.00	108.05	106.00
76.05	767.00	87.05	109.00	98.00	23.00	109.05	135.00
77.05	7206.00	88.00	46.00	99.05	12.00	110.05	12.00
78.05	3559.00	89.05	1390.00	100.00	1.00	111.05	2.00
79.05	1322.00	90.05	706.00	101.05	54.00	111.85	1.00
80.05	180.00	91.05	9999.00	102.05	406.00	114.00	1.00
81.05	433.00	92.05	2197.00	103.05	2318.00	115.05	4.00
82.00	55.00	93.05	3949.00	104.05	9291.00	116.05	14.00
83.05	20.00	94.05	1204.00	105.05	1782.00	117.05	24.00
84.00	8.00	95.05	135.00	106.05	560.00	118.05	350.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
119.05	1422.00	131.00	459.00	143.20	1.00	163.15	1.00
120.05	523.00	132.05	1031.00	144.05	1.00	164.05	14.00
121.05	408.00	133.05	188.00	145.05	1.00	165.05	3.00
122.05	166.00	134.05	235.00	146.05	30.00	166.05	26.00

123.05	49.00	135.05	334.00	147.05	10.00	167.05	12.00
124.05	22.00	136.05	36.00	148.05	468.00	168.10	4.00
125.10	2.00	137.05	9.00	149.05	1039.00	169.00	1.00
126.05	1.00	138.05	12.00	150.00	292.00	180.05	1.00
127.05	1.00	139.05	1.00	151.05	30.00	181.00	1.00
128.15	1.00	140.95	1.00	152.05	16.00	207.00	1.00
130.05	274.00	142.05	1.00	153.05	3.00		

#76: 2,5-DIMETHYLFURAN
Modified: scaled

Entry Number 76 from C:\DATABASE\hjf.l
CAS 000625-86-5
Melting Point -300
Boiling Point -300
Retention Index 16.3
Mol Formula C6H8O
Mol Weight 96.057

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	201.00	39.95	64.00	52.00	531.00	65.00	319.00
26.90	760.00	40.95	436.00	53.00	4138.00	66.00	57.00
27.90	12.00	41.95	254.00	54.00	290.00	67.05	718.00
33.30	2.00	42.90	6023.00	54.95	125.00	68.00	51.00
33.55	5.00	44.90	8.00	56.00	14.00	68.90	17.00
33.90	6.00	45.95	3.00	57.00	2.00	71.00	10.00
34.40	2.00	46.95	73.00	59.95	3.00	72.00	2.00
35.85	20.00	47.85	47.00	60.90	21.00	72.95	8.00
36.90	63.00	48.90	110.00	61.95	25.00	74.00	19.00
37.90	92.00	49.90	720.00	62.95	22.00	74.95	8.00
38.90	338.00	50.90	1049.00	64.05	7.00	76.00	2.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
77.05	153.00	88.30	2.00	105.05	8.00		
78.00	25.00	90.05	2.00	111.90	3.00		
78.95	290.00	91.00	1.00	119.00	3.00		
80.05	159.00	92.05	2.00	150.00	3.00		
81.05	725.00	92.95	7.00	219.95	2.00		
82.00	52.00	94.00	219.00				
83.05	5.00	95.05	8094.00				
83.90	1.00	96.05	9999.00				
85.95	14.00	97.05	637.00				
86.85	2.00	98.05	39.00				
87.15	2.00	103.90	2.00				

#77: 3,5-DIMETHYLPHENOL
Modified: scaled

Entry Number 77 from C:\DATABASE\hjf.l
CAS 000108-68-9
Melting Point -300
Boiling Point -300
Retention Index 67.7
Mol Formula C8H10O
Mol Weight 122.072

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	43.00	39.90	126.00	52.00	293.00	62.95	277.00
26.90	455.00	40.90	291.00	52.95	566.00	64.05	71.00
28.90	80.00	41.90	47.00	54.00	65.00	65.00	509.00
29.95	1.00	43.05	114.00	54.95	236.00	66.00	159.00
30.90	8.00	44.90	43.00	55.95	10.00	67.05	176.00
32.95	3.00	45.90	68.00	57.00	5.00	68.05	25.00
34.85	0.00	46.90	15.00	57.95	1.00	68.90	7.00
35.90	3.00	47.85	4.00	59.05	86.00	69.95	1.00
36.90	51.00	48.90	28.00	60.05	383.00	70.95	0.00
37.90	170.00	49.90	297.00	60.90	136.00	71.95	1.00
38.90	922.00	50.90	686.00	61.90	119.00	72.90	16.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
73.95	81.00	84.95	13.00	96.05	6.00	109.05	44.00
74.95	60.00	86.00	20.00	96.95	3.00	110.05	2.00
76.00	57.00	87.05	18.00	98.05	10.00	117.05	2.00
77.05	2281.00	88.00	5.00	99.05	3.00	118.05	7.00
78.05	538.00	89.05	71.00	101.00	12.00	119.00	48.00
79.05	1480.00	90.05	12.00	102.05	54.00	121.05	3396.00
80.05	123.00	91.05	1337.00	103.05	328.00	122.05	9999.00
81.05	84.00	92.00	148.00	104.05	211.00	123.05	890.00
82.05	35.00	93.05	366.00	105.05	251.00	124.05	56.00
83.05	22.00	94.05	215.00	107.05	9120.00	125.05	3.00
83.95	2.00	95.00	46.00	108.05	700.00	131.90	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
135.10	1.00						
137.95	0.00						
138.20	0.00						
149.80	0.00						
158.05	1.00						
166.15	2.00						
169.00	0.00						
181.00	0.00						
184.05	0.00						

#78: 1-(4-METHYLPHENYL)-PROPANONE
Modified: scaled

Entry Number 78 from C:\DATABASE\hjf.l
CAS 005337-93-9
Melting Point -300
Boiling Point -300
Retention Index 69.5
Mol Formula C10H12O
Mol Weight 148.088
Miscellaneous Information
Aldrich: 4'-methylpropiophenone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	26.00	41.95	10.00	56.00	8.00	67.00	3.00
26.90	191.00	47.80	0.00	57.05	50.00	67.90	0.00
28.90	186.00	47.90	0.00	57.85	5.00	70.95	1.00
30.00	3.00	48.05	0.00	59.00	10.00	72.00	7.00
32.90	0.00	48.95	5.00	59.85	3.00	73.00	9.00
35.95	1.00	49.90	116.00	60.90	23.00	73.95	35.00
36.90	13.00	50.90	220.00	61.90	99.00	74.95	33.00
37.90	47.00	51.95	47.00	63.05	332.00	76.05	27.00
38.90	471.00	52.90	38.00	64.05	108.00	77.00	97.00
39.90	36.00	54.05	3.00	65.05	1395.00	78.00	30.00
40.95	146.00	54.90	68.00	66.05	82.00	79.05	23.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
80.00	2.00	91.05	4398.00	103.05	37.00	116.00	10.00
81.00	0.00	92.05	349.00	104.05	17.00	117.05	23.00
82.05	0.00	93.05	19.00	105.05	34.00	119.05	9999.00
83.00	0.00	94.05	1.00	106.05	4.00	120.05	910.00
83.90	0.00	95.00	0.00	109.00	1.00	121.05	55.00
85.00	8.00	95.80	0.00	110.05	1.00	122.05	1.00
86.00	22.00	97.00	1.00	111.05	0.00	126.05	2.00
87.05	21.00	98.00	3.00	111.90	0.00	127.05	5.00
88.00	7.00	99.05	1.00	113.05	1.00	128.05	8.00
89.05	394.00	101.05	3.00	113.95	0.00	129.05	6.00
90.05	216.00	102.05	13.00	115.05	41.00	130.10	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
131.00	22.00	147.15	26.00				
132.05	6.00	148.05	1345.00				
133.05	71.00	149.05	146.00				
134.05	7.00	150.00	9.00				
135.10	1.00	151.10	1.00				
141.05	0.00	181.05	0.00				
142.15	1.00	239.15	0.00				
143.20	0.00						
144.05	1.00						
145.05	2.00						
146.05	5.00						

#79: 2-ETHYLFURAN
Modified: scaled

Entry Number 79 from C:\DATABASE\hjf.l
CAS 003208-16-0
Melting Point -300
Boiling Point -300
Retention Index 16
Mol Formula C6H8O
Mol Weight 96.057

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	125.00	36.10	9.00	48.15	6.00	58.95	2.00
26.95	756.00	36.90	136.00	48.90	36.00	59.95	7.00
27.90	129.00	37.90	324.00	49.90	227.00	60.95	46.00
28.90	282.00	38.90	1331.00	50.90	384.00	62.00	99.00
29.95	3.00	39.90	266.00	51.95	230.00	62.95	172.00
30.90	7.00	40.95	882.00	53.00	2815.00	64.00	50.00
32.85	1.00	41.95	157.00	54.00	158.00	65.00	503.00
33.15	7.00	43.05	35.00	55.00	119.00	66.00	185.00
33.55	3.00	45.90	4.00	56.00	3.00	67.05	619.00
34.05	6.00	46.95	26.00	57.00	26.00	68.00	166.00
35.85	15.00	47.80	7.00	57.65	3.00	68.90	3.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
70.00	4.00	83.05	42.00	99.95	2.00		
71.00	9.00	83.90	4.00	105.05	40.00		
72.00	3.00	88.05	5.00	112.05	3.00		
72.95	9.00	89.00	2.00	113.95	3.00		
73.95	10.00	92.05	5.00	149.95	9.00		
75.00	9.00	92.95	4.00	218.95	6.00		
77.05	77.00	93.95	102.00				
78.00	12.00	95.05	638.00				
78.95	32.00	96.05	4175.00				
81.05	9999.00	97.05	284.00				
82.00	588.00	98.05	24.00				

#80: NITROBENZENE
Modified: scaled
Entry Number 80 from C:\DATABASE\hjf.l
CAS 000098-95-3
Melting Point -300
Boiling Point -300
Retention Index 57.07
Mol Formula C6H5NO2
Mol Weight 123.031

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	54.00	42.00	3.00	57.85	0.00	69.95	0.00
26.90	277.00	45.90	9.00	58.55	0.00	70.90	0.00
29.90	721.00	47.90	11.00	59.90	14.00	71.95	7.00
30.90	1.00	48.90	120.00	60.90	62.00	72.95	107.00
32.95	1.00	49.90	1578.00	61.90	84.00	73.90	513.00
35.95	17.00	50.90	4755.00	62.95	161.00	75.00	325.00
36.90	179.00	51.95	232.00	64.05	114.00	76.05	342.00
37.90	249.00	52.90	19.00	65.05	1347.00	77.05	9999.00
38.90	503.00	53.90	2.00	66.05	85.00	78.05	678.00
39.90	25.00	54.95	3.00	67.00	4.00	79.00	18.00
40.90	10.00	56.00	1.00	67.95	1.00	79.95	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
80.90	1.00	103.00	1.00	120.90	0.00		
86.00	3.00	103.90	0.00	121.10	0.00		
87.00	7.00	104.10	1.00	123.05	6283.00		
88.00	5.00	105.05	2.00	124.05	463.00		
88.95	2.00	107.05	159.00	125.05	39.00		
90.05	5.00	108.00	11.00	126.00	3.00		
91.05	17.00	109.00	2.00	128.00	1.00		
93.05	1396.00	115.00	1.00	142.95	0.00		
94.05	92.00	116.05	1.00	154.10	3.00		
95.00	5.00	117.10	1.00	156.10	2.00		
96.00	1.00	120.05	0.00	180.95	0.00		

#81: 3-ETHYLBENZOIC ACID
Modified: scaled

Entry Number 81 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 80.9
Mol Formula C9H10O2
Mol Weight 150.068

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	32.00	39.90	57.00	55.00	55.00	72.00	3.00
27.00	414.00	41.00	73.00	58.95	24.00	73.00	48.00
28.90	26.00	42.00	8.00	59.95	28.00	74.00	223.00
29.95	3.00	44.90	154.00	60.95	54.00	75.00	217.00
34.10	4.00	47.95	6.00	61.95	181.00	76.00	216.00
34.85	2.00	49.00	38.00	62.95	538.00	77.05	2482.00
35.95	9.00	49.90	478.00	64.05	142.00	78.05	574.00
36.30	3.00	50.90	1124.00	65.00	456.00	79.05	1529.00
36.95	34.00	51.95	211.00	65.95	98.00	80.00	104.00
37.90	115.00	52.95	283.00	66.95	13.00	81.05	23.00
38.90	624.00	54.00	17.00	68.00	5.00	84.05	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
85.05	13.00	95.95	4.00	108.05	177.00	123.00	21.00
86.00	36.00	98.00	25.00	109.00	18.00	123.95	5.00
87.00	48.00	99.05	7.00	110.10	6.00	127.10	3.00
88.05	23.00	100.00	2.00	115.00	7.00	129.05	14.00
89.00	590.00	101.05	55.00	116.05	3.00	130.05	1.00
90.05	354.00	102.05	177.00	117.05	20.00	131.00	201.00
91.05	1915.00	103.05	1082.00	118.05	52.00	132.05	120.00
92.05	166.00	104.05	334.00	119.05	28.00	133.05	520.00
93.00	17.00	105.05	9999.00	120.05	14.00	135.05	5308.00
94.00	13.00	106.05	1120.00	121.05	14.00	136.05	494.00
95.05	6.00	107.05	2397.00	122.05	76.00	137.05	49.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
138.05	12.00	169.05	0.00				
141.10	1.00	181.05	1.00				
147.10	4.00	218.95	3.00				
148.05	40.00						
149.05	103.00						
150.05	6076.00						
151.05	598.00						
152.05	55.00						
153.10	6.00						
154.20	1.00						
164.05	3.00						

#82: 3-METHYL-4-NITROBENZYL ALCOHOL
Modified: scaled

Entry Number 82 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 81.829
Mol Formula C8H9NO3
Mol Weight 167.057

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	59.00	38.90	2073.00	53.90	50.00	64.00	722.00
27.05	443.00	39.90	167.00	54.95	349.00	65.05	6685.00
28.90	651.00	40.95	524.00	56.00	27.00	66.00	501.00
29.90	257.00	42.00	66.00	57.05	1014.00	67.05	247.00
33.30	6.00	46.95	4.00	57.95	45.00	68.00	43.00
34.70	1.00	47.95	13.00	59.00	18.00	70.00	8.00
35.00	2.00	48.90	57.00	59.65	18.00	71.05	29.00
35.85	6.00	49.95	578.00	59.90	3.00	72.10	15.00
36.05	2.00	50.95	1185.00	60.95	200.00	73.05	97.00
36.85	120.00	52.00	349.00	61.95	638.00	74.00	262.00
37.90	314.00	53.00	359.00	63.00	2041.00	75.00	276.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
76.00	156.00	87.00	143.00	98.05	20.00	109.05	75.00
77.05	1766.00	88.05	72.00	99.05	21.00	110.15	15.00
78.05	488.00	89.05	2131.00	99.95	6.00	111.05	12.00
79.05	502.00	90.05	974.00	101.00	17.00	112.05	8.00
80.00	117.00	91.05	2762.00	102.00	37.00	113.15	10.00
81.00	114.00	92.05	3406.00	103.05	77.00	114.00	4.00
82.05	31.00	93.00	555.00	104.05	91.00	115.10	9.00
83.05	11.00	94.05	63.00	105.05	164.00	116.05	21.00
83.95	18.00	95.05	363.00	106.05	924.00	117.05	396.00
85.05	91.00	96.00	81.00	107.05	406.00	118.00	689.00
85.95	175.00	97.10	23.00	108.05	103.00	119.00	383.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
120.05	768.00	135.05	718.00	153.10	19.00	176.05	4.00
121.00	236.00	136.05	92.00	160.05	4.00	178.20	4.00
122.05	110.00	137.05	20.00	161.15	8.00	180.95	7.00
123.05	1142.00	138.05	4.00	162.20	4.00	190.10	18.00
124.05	112.00	144.95	8.00	163.05	4.00	206.05	4.00
125.10	14.00	146.05	67.00	164.00	163.00	208.15	303.00
128.15	4.00	148.05	9999.00	165.05	872.00	209.10	49.00
131.00	4.00	149.05	946.00	166.05	101.00	210.20	4.00
132.05	17.00	150.05	67.00	167.15	18.00	219.95	1.00
133.05	38.00	151.05	1284.00	169.00	5.00		
134.05	849.00	152.05	159.00	175.10	31.00		

#83: 3,5-DIMETHYLPYRAZOLE
Modified: scaled

Entry Number 83 from C:\DATABASE\hjf.l
CAS 000067-51-6
Melting Point -300
Boiling Point -300
Retention Index 54.46
Mol Formula C5H8N2
Mol Weight 96.069

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	172.00	35.30	1.00	50.90	225.00	62.95	164.00
27.05	475.00	35.95	12.00	51.90	283.00	64.00	47.00
27.90	898.00	36.90	94.00	52.95	213.00	65.00	516.00
28.90	159.00	37.90	209.00	54.00	1868.00	66.00	194.00
29.90	189.00	38.90	1253.00	55.05	543.00	67.05	293.00
30.90	24.00	39.90	419.00	56.05	223.00	68.05	663.00
31.90	206.00	40.90	1131.00	58.40	1.00	68.95	129.00
33.90	1.00	41.95	1040.00	58.95	4.00	73.15	1.00
34.60	2.00	46.95	146.00	60.00	12.00	73.80	1.00
34.85	5.00	48.90	22.00	60.90	46.00	74.95	6.00
35.05	2.00	49.90	96.00	61.90	93.00	75.95	8.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
77.00	11.00	96.05	9999.00	118.95	2.00		
78.00	130.00	97.05	639.00	120.00	7.00		
79.00	74.00	98.05	11.00	121.00	3.00		
80.05	36.00	104.05	1.00	131.95	2.00		
81.05	1358.00	104.90	1.00	180.95	1.00		
82.05	79.00	105.10	5.00				
83.05	7.00	108.05	1.00				
88.55	1.00	111.05	4.00				
91.05	6.00	114.00	0.00				
93.00	11.00	115.05	1.00				
95.05	7728.00	117.10	4.00				

#84: 3,5-DIMETHYLPYRAZOLE
Modified: scaled

Entry Number 84 from C:\DATABASE\hjf.l
CAS 000108-39-4
Melting Point -300
Boiling Point -300
Retention Index 62.06
Mol Formula C7H8O

Mol Weight 108.057

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.85	72.00	41.90	61.00	55.95	8.00	65.95	153.00
26.90	502.00	46.80	1.00	57.00	4.00	66.95	90.00
28.90	73.00	46.90	0.00	58.10	2.00	68.00	85.00
32.95	0.00	47.95	6.00	58.40	0.00	68.90	31.00
34.30	0.00	48.90	51.00	58.65	0.00	70.00	2.00
35.90	9.00	49.90	397.00	59.90	13.00	71.05	0.00
36.90	124.00	50.90	754.00	60.90	82.00	71.90	3.00
37.90	333.00	52.00	395.00	61.90	179.00	72.90	29.00
38.90	1190.00	52.90	765.00	62.90	426.00	73.90	103.00
39.90	194.00	53.90	428.00	64.00	126.00	75.00	50.00
40.95	116.00	54.90	207.00	65.00	270.00	76.00	17.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
77.05	2338.00	88.05	1.00	102.15	0.00	117.05	0.00
78.05	488.00	89.00	393.00	103.00	2.00	121.05	1.00
79.05	2700.00	90.05	1152.00	104.05	0.00	122.10	1.00
80.05	1020.00	91.05	537.00	105.00	65.00	128.15	0.00
81.00	156.00	92.05	47.00	107.05	8532.00	145.05	0.00
82.05	27.00	93.00	21.00	108.05	9999.00	152.05	1.00
83.05	2.00	94.00	4.00	109.05	773.00	165.10	1.00
83.95	8.00	95.05	1.00	110.05	47.00	167.05	2.00
84.95	21.00	96.05	1.00	111.10	3.00		
86.00	29.00	97.00	1.00	115.05	0.00		
87.00	23.00	101.00	2.00	115.90	0.00		

#85: 2,5-DIMETHYLBENZOIC ACID
Modified: scaled

Entry Number 85 from C:\DATABASE\hjf.l
CAS 000611-01-8
Melting Point -300
Boiling Point -300
Retention Index 79.569
Mol Formula C9H10O2
Mol Weight 150.068

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	39.00	46.95	4.00	57.00	11.00	70.00	4.00
26.90	523.00	47.65	3.00	57.95	10.00	71.00	8.00
28.90	16.00	47.95	0.00	59.00	69.00	72.05	4.00
35.85	8.00	48.95	40.00	59.95	28.00	73.00	36.00
36.95	62.00	49.95	449.00	60.90	85.00	74.00	240.00
37.90	178.00	50.95	1821.00	61.90	274.00	74.90	203.00
38.90	1085.00	51.90	494.00	62.95	703.00	76.05	206.00
39.90	95.00	52.95	539.00	64.00	166.00	77.05	2983.00

40.95	201.00	54.00	38.00	65.00	753.00	78.05	1698.00
42.00	24.00	54.95	76.00	65.90	865.00	79.05	1927.00
44.90	63.00	56.05	8.00	67.95	12.00	80.00	120.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
81.00	19.00	92.05	146.00	104.05	5305.00	117.05	8.00
82.00	6.00	93.00	99.00	105.05	5984.00	118.00	18.00
83.00	6.00	94.00	17.00	106.05	548.00	119.00	122.00
84.00	8.00	95.05	13.00	107.05	195.00	120.05	19.00
85.00	30.00	96.05	12.00	108.05	17.00	121.05	159.00
85.95	58.00	97.00	12.00	109.05	7.00	122.00	34.00
87.00	68.00	98.05	39.00	110.05	1.00	122.95	4.00
88.00	25.00	98.95	12.00	111.15	1.00	123.10	3.00
89.00	271.00	101.05	49.00	112.05	1.00	129.05	11.00
90.05	93.00	102.00	290.00	115.05	5.00	130.05	3.00
91.05	1729.00	103.05	1953.00	116.05	7.00	131.00	41.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
132.05	9999.00	150.05	8890.00				
133.05	3685.00	151.05	878.00				
134.05	337.00	152.05	81.00				
135.05	348.00	153.10	7.00				
136.05	39.00	162.20	1.00				
137.05	9.00	164.05	1.00				
138.05	1.00	169.00	1.00				
143.05	1.00	180.95	1.00				
147.05	28.00						
148.05	30.00						
149.05	253.00						

#86: 3-NITROBENZENE METHANOL
Modified: scaled

Entry Number 86 from C:\DATABASE\hjf.l
CAS 000619-25-0
Melting Point -300
Boiling Point -300
Retention Index 86.629
Mol Formula C7H7NO3
Mol Weight 153.042
Miscellaneous Information
Aldrich: 3-nitrobenzyl alcohol

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	82.00	38.90	1514.00	53.00	1081.00	65.00	406.00
26.90	741.00	39.90	179.00	54.90	260.00	66.00	257.00
28.90	541.00	40.95	326.00	56.05	13.00	67.00	178.00
29.90	428.00	41.95	38.00	57.05	4.00	68.00	48.00
30.90	703.00	45.90	30.00	58.00	0.00	70.00	1.00

32.95	1.00	46.90	5.00	58.90	0.00	71.05	2.00
33.95	0.00	47.85	10.00	59.95	17.00	72.05	6.00
34.70	1.00	48.90	95.00	60.90	143.00	72.90	93.00
35.90	9.00	49.90	1682.00	61.95	406.00	73.95	564.00
36.90	165.00	50.90	3596.00	63.00	1527.00	75.00	525.00
37.90	360.00	51.95	911.00	64.00	407.00	76.05	1030.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
77.05	9999.00	89.05	6433.00	101.00	3.00	112.00	1.00
78.05	3603.00	90.00	1018.00	102.05	3.00	115.05	1.00
79.05	1270.00	91.05	181.00	103.05	14.00	116.00	2.00
80.05	95.00	92.05	191.00	104.05	203.00	117.05	2.00
81.05	41.00	93.05	70.00	105.05	2433.00	118.05	3.00
82.05	5.00	94.05	526.00	106.05	4278.00	119.00	2.00
83.05	3.00	95.05	93.00	107.05	3637.00	120.00	40.00
83.95	8.00	96.05	7.00	108.05	2323.00	121.05	281.00
85.05	38.00	97.05	1.00	109.05	164.00	122.05	98.00
86.00	81.00	98.10	1.00	110.00	12.00	123.05	141.00
87.00	82.00	99.05	3.00	111.05	2.00	124.05	831.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
125.00	165.00	137.05	613.00	152.05	745.00	169.00	1.00
126.00	14.00	138.05	56.00	153.05	4465.00	176.00	0.00
127.05	2.00	139.05	10.00	154.00	475.00	178.05	2.00
128.05	3.00	140.05	2.00	155.05	106.00	181.10	2.00
129.05	3.00	141.10	2.00	156.05	9.00	182.05	1.00
130.05	3.00	143.05	1.00	157.15	1.00	183.05	2.00
132.05	11.00	145.05	0.00	163.05	2.00	184.05	2.00
133.05	8.00	147.05	2.00	164.00	2.00	186.05	3.00
134.05	17.00	148.05	2.00	166.00	2.00	193.00	0.00
135.05	78.00	150.05	206.00	167.05	4.00	194.10	2.00
136.05	4815.00	151.05	104.00	168.10	3.00	195.05	1.00

#87: 5-METHYL-2(3H)-FURANONE
Modified: scaled

Entry Number 87 from C:\DATABASE\hjf.l
CAS 000591-12-8
Melting Point -300
Boiling Point -300
Retention Index 39.77
Mol Formula C5H6O2
Mol Weight 98.037
Miscellaneous Information
Aldrich: alpha-angelicalactone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	893.00	36.90	172.00	51.95	148.00	61.95	2.00
26.90	2497.00	37.85	215.00	52.90	475.00	62.95	1.00

27.90	262.00	38.90	1041.00	54.05	449.00	63.80	2.00
28.90	146.00	39.90	178.00	54.90	9999.00	64.10	3.00
29.95	3.00	41.00	505.00	55.95	426.00	64.95	3.00
30.90	20.00	41.90	1336.00	56.95	30.00	65.95	6.00
32.90	3.00	42.95	6738.00	58.05	2.00	67.00	5.00
33.90	8.00	47.90	16.00	58.80	1.00	68.05	46.00
34.65	2.00	48.90	109.00	59.15	1.00	68.95	313.00
34.85	5.00	49.90	327.00	59.95	3.00	70.05	1234.00
35.90	31.00	50.90	251.00	60.95	6.00	71.05	60.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
72.00	6.00	90.95	2.00	105.05	9.00		
72.80	1.00	92.90	1.00	106.05	1.00		
76.95	3.00	93.90	1.00	120.10	3.00		
77.95	2.00	96.05	69.00	149.95	2.00		
78.95	15.00	97.05	27.00	219.95	0.00		
79.95	5.00	98.05	9379.00				
80.40	1.00	99.05	542.00				
81.00	3.00	100.00	50.00				
81.90	220.00	101.05	6.00				
82.95	88.00	102.55	1.00				
83.95	7.00	103.05	1.00				

#88: 4-NITROTOLUENE
Modified: scaled

Entry Number 88 from C:\DATABASE\hjf.l
CAS 000099-99-0
Melting Point -300
Boiling Point -300
Retention Index 66.689
Mol Formula C7H7NO2
Mol Weight 137.048

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	68.00	39.90	160.00	54.90	8.00	64.00	432.00
26.90	238.00	40.95	525.00	56.00	1.00	65.00	7437.00
28.90	2.00	42.05	22.00	56.30	0.00	66.00	408.00
29.90	439.00	45.90	20.00	56.95	1.00	67.00	14.00
33.40	0.00	47.95	7.00	57.30	0.00	67.75	0.00
33.95	1.00	48.90	64.00	58.55	0.00	67.90	1.00
34.65	0.00	49.90	721.00	59.05	0.00	68.05	2.00
35.95	7.00	50.90	1005.00	59.95	17.00	71.95	3.00
36.90	120.00	51.95	298.00	60.90	178.00	72.90	32.00
37.90	306.00	52.95	210.00	61.90	544.00	73.90	185.00
38.90	2308.00	53.95	14.00	62.90	1612.00	74.95	154.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
76.00	104.00	86.95	100.00	97.95	1.00	110.10	1.00

77.00	1521.00	88.05	36.00	98.95	4.00	110.40	0.00
78.00	304.00	89.05	1361.00	101.00	0.00	115.00	1.00
79.05	1423.00	90.00	416.00	102.05	3.00	116.10	2.00
80.05	99.00	91.05	9999.00	103.00	4.00	117.00	2.00
80.95	6.00	92.05	779.00	104.00	27.00	118.00	3.00
82.05	1.00	93.00	27.00	105.00	18.00	119.00	0.00
83.15	0.00	94.05	2.00	106.00	93.00	120.05	18.00
83.95	16.00	95.05	1.00	107.05	2509.00	121.05	206.00
84.90	66.00	95.30	0.00	108.05	198.00	122.05	21.00
85.95	131.00	96.00	1.00	109.00	13.00	123.05	3.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
128.15	0.00	182.05	0.00				
131.95	2.00	219.95	0.00				
133.00	2.00						
135.05	16.00						
137.05	9548.00						
138.05	788.00						
139.05	67.00						
140.00	4.00						
145.05	0.00						
156.10	2.00						
181.00	0.00						

#89: 2,5-DIMETHYLBENZOIC ACID
Modified: scaled

Entry Number 89 from C:\DATABASE\hjf.l
CAS 000610-72-0
Melting Point -300
Boiling Point -300
Retention Index 79.219
Mol Formula C9H10O2
Mol Weight 150.068

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	59.00	38.90	1235.00	52.90	694.00	65.00	909.00
26.95	765.00	39.90	124.00	53.95	60.00	65.90	1120.00
28.90	94.00	40.95	256.00	54.95	87.00	66.95	3.00
29.90	6.00	41.95	34.00	57.65	3.00	67.95	7.00
32.95	14.00	44.90	165.00	57.90	4.00	69.95	3.00
33.70	8.00	47.65	3.00	58.95	131.00	71.90	3.00
34.05	3.00	47.85	6.00	59.90	70.00	72.95	80.00
35.85	22.00	48.90	60.00	60.90	126.00	73.95	337.00
36.05	6.00	49.85	651.00	61.90	321.00	74.90	295.00
36.95	84.00	50.90	2598.00	62.95	835.00	76.00	272.00
37.95	208.00	51.90	697.00	63.95	205.00	76.95	3952.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.

78.00	2225.00	85.95	103.00	96.10	31.00	107.00	264.00
79.00	2406.00	87.00	94.00	96.95	31.00	108.00	42.00
80.05	182.00	87.95	50.00	97.95	63.00	109.05	20.00
81.00	42.00	88.95	351.00	99.00	14.00	110.05	3.00
82.00	25.00	90.05	134.00	99.95	1.00	114.00	10.00
83.10	18.00	91.00	2328.00	101.00	96.00	115.05	6.00
83.55	4.00	92.00	226.00	102.05	373.00	116.00	10.00
83.80	4.00	93.00	179.00	103.05	2659.00	117.05	27.00
83.90	18.00	94.00	38.00	104.05	8851.00	117.90	8.00
84.05	11.00	95.00	35.00	105.05	8326.00	118.10	22.00
85.00	18.00	95.90	4.00	106.05	852.00	118.95	159.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
120.00	35.00	147.05	57.00				
121.00	73.00	148.05	53.00				
122.00	50.00	149.05	401.00				
129.00	21.00	150.00	9999.00				
130.95	346.00	151.05	1014.00				
132.05	9681.00	152.05	116.00				
133.05	2251.00	164.00	7.00				
134.05	219.00	168.95	11.00				
135.05	799.00	180.95	3.00				
136.05	108.00	220.05	3.00				
137.00	29.00						

#90: 3-METHYL-4-NITROPHENOL
Modified: scaled

Entry Number 90 from C:\DATABASE\hjf.l
CAS 002581-34-2
Melting Point -300
Boiling Point -300
Retention Index 89.5
Mol Formula C7H7NO3
Mol Weight 153.042

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	127.00	37.90	512.00	50.90	2063.00	60.95	156.00
26.95	1093.00	38.90	1938.00	51.90	1734.00	61.90	438.00
28.90	204.00	39.90	283.00	52.90	2723.00	62.90	1007.00
29.90	402.00	40.90	734.00	53.90	381.00	63.95	271.00
30.90	21.00	41.95	151.00	54.90	1713.00	64.90	1124.00
34.15	9.00	45.90	5.00	56.00	101.00	65.90	503.00
34.40	5.00	46.90	29.00	57.00	124.00	66.95	978.00
34.80	3.00	47.80	19.00	57.80	9.00	67.90	742.00
35.10	9.00	48.05	17.00	57.90	34.00	68.90	110.00
35.90	10.00	48.90	86.00	58.95	3.00	70.00	43.00
36.85	180.00	49.90	773.00	59.90	31.00	71.05	84.00

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
71.95	21.00	83.00	57.00	94.00	417.00	105.95	326.00
72.95	89.00	84.00	38.00	95.00	225.00	107.00	679.00
73.90	258.00	85.05	79.00	95.95	125.00	108.00	1206.00
74.90	168.00	85.95	65.00	97.00	33.00	108.95	701.00
75.95	184.00	86.90	58.00	98.00	12.00	110.05	103.00
76.90	6379.00	87.95	40.00	99.05	34.00	111.00	27.00
77.95	1271.00	88.95	124.00	100.95	7.00	111.90	17.00
78.95	974.00	89.90	490.00	101.95	17.00	112.05	12.00
79.95	2347.00	90.95	156.00	103.00	40.00	113.05	5.00
80.90	2014.00	91.90	241.00	104.00	86.00	113.95	7.00
81.95	273.00	92.95	198.00	105.00	354.00	114.95	14.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
116.00	17.00	126.80	7.00	138.00	120.00	152.95	4419.00
116.95	5.00	127.05	14.00	139.10	36.00	154.00	380.00
118.00	45.00	128.10	15.00	140.00	15.00	155.00	67.00
118.90	40.00	128.95	10.00	141.00	19.00	155.80	7.00
120.05	52.00	130.90	12.00	144.95	2.00	156.05	7.00
121.00	108.00	132.00	36.00	146.95	21.00	160.95	7.00
122.00	347.00	133.00	33.00	147.95	12.00	163.00	7.00
123.00	771.00	134.00	22.00	149.05	19.00	163.95	36.00
124.00	117.00	135.05	228.00	150.00	48.00	165.00	12.00
125.00	19.00	136.00	9999.00	151.00	27.00	165.95	24.00
126.10	36.00	137.00	1041.00	151.95	9.00	167.00	36.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
168.95	7.00						
175.05	7.00						
176.05	3.00						
180.95	3.00						
190.95	9.00						
191.95	7.00						
192.90	29.00						
206.95	26.00						
207.95	15.00						
208.90	15.00						
218.95	22.00						

#91: 2,5-DIHYDRO-2,5-DIMETHOXY-2-METHYLFURAN
Modified: scaled

Entry Number 91 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 37.92
Mol Formula C7H12O3
Mol Weight 144.078

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	142.00	35.90	1.00	48.00	1.00	58.90	948.00
26.90	712.00	36.90	30.00	48.90	8.00	59.95	23.00
27.90	122.00	37.90	87.00	49.95	88.00	60.95	18.00
28.90	766.00	38.90	907.00	50.90	162.00	61.90	4.00
29.90	54.00	39.95	184.00	52.00	102.00	62.95	5.00
30.90	186.00	40.95	877.00	53.05	2295.00	64.05	6.00
31.90	48.00	42.05	508.00	54.00	507.00	64.30	1.00
32.95	70.00	42.90	2154.00	55.05	2218.00	65.00	15.00
33.95	0.00	44.95	541.00	56.05	112.00	65.95	6.00
34.30	0.00	45.95	11.00	57.00	151.00	67.05	18.00
35.00	1.00	46.95	22.00	58.00	30.00	68.00	106.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
69.00	462.00	82.05	321.00	93.95	1.00	111.05	924.00
70.00	256.00	83.05	559.00	95.05	32.00	112.05	295.00
71.05	957.00	84.00	113.00	96.05	11.00	113.05	9999.00
72.00	44.00	85.05	1829.00	97.05	203.00	114.05	667.00
73.05	7.00	86.00	104.00	98.05	109.00	115.05	87.00
74.00	4.00	87.05	26.00	99.05	23.00	116.05	6.00
75.05	40.00	88.00	3.00	101.05	1190.00	117.05	0.00
76.05	3.00	89.05	6.00	102.05	67.00	127.05	4.00
77.00	2.00	89.90	1.00	103.05	8.00	129.05	1176.00
79.00	165.00	91.00	1.00	104.05	0.00	130.05	77.00
81.05	3518.00	92.95	1.00	109.15	0.00	131.00	2.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
131.95	1.00						
143.05	491.00						
144.05	39.00						
145.10	5.00						

#92: 2-METHOXYPHENOL
Modified: scaled

Entry Number 92 from C:\DATABASE\hjf.l
CAS 000090-05-1
Melting Point -300
Boiling Point -300
Retention Index 56.81
Mol Formula C7H8O2
Mol Weight 124.052
Miscellaneous Information
Aldrich: guaiacol

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	222.00	36.90	114.00	52.90	1544.00	63.90	180.00
26.90	776.00	37.90	275.00	53.90	157.00	64.90	491.00

28.90	171.00	38.90	768.00	54.90	235.00	65.90	106.00
29.90	12.00	39.90	70.00	55.90	11.00	66.90	87.00
30.90	60.00	40.90	140.00	56.85	3.00	67.95	15.00
32.95	0.00	41.90	50.00	58.00	1.00	68.90	14.00
33.65	0.00	47.55	11.00	58.90	2.00	69.90	2.00
33.85	0.00	48.90	62.00	59.85	11.00	70.85	2.00
34.30	1.00	49.90	414.00	60.90	70.00	71.85	1.00
34.80	0.00	50.90	653.00	61.90	188.00	72.90	12.00
35.95	8.00	51.90	739.00	62.90	434.00	73.90	51.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
74.90	31.00	88.15	0.00	100.90	0.00	114.90	1.00
75.90	35.00	88.95	1.00	101.30	0.00	115.15	0.00
76.90	321.00	89.90	4.00	102.95	1.00	117.05	1.00
77.90	49.00	90.95	7.00	104.00	3.00	120.90	35.00
78.90	116.00	91.90	48.00	104.95	6.00	121.95	11.00
80.00	174.00	92.90	56.00	106.00	3.00	124.00	9083.00
80.90	4404.00	94.00	29.00	106.90	13.00	124.95	721.00
81.90	247.00	95.00	166.00	108.90	9999.00	126.00	63.00
82.90	16.00	96.05	32.00	109.90	672.00	127.00	4.00
83.95	2.00	97.00	3.00	110.90	60.00	142.95	0.00
84.80	0.00	98.00	0.00	112.00	4.00	144.95	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
150.05	0.00						
168.95	0.00						

#93: DIHYDRO-2,5-FURANDIONE
Modified: scaled

Entry Number 93 from C:\DATABASE\hjf.l
CAS 000108-30-5
Melting Point -300
Boiling Point -300
Retention Index 64.45
Mol Formula C4H4O3
Mol Weight 100.016
Miscellaneous Information
Aldrich: succinic anhydride

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	2053.00	39.90	15.00	55.00	295.00	68.90	3.00
26.95	2000.00	40.95	113.00	55.95	5259.00	78.00	3.00
27.90	9999.00	41.90	501.00	57.00	175.00	79.05	4.00
28.90	481.00	44.90	46.00	57.95	13.00	80.00	3.00
29.95	9.00	45.90	11.00	59.05	1.00	85.90	1.00
32.95	4.00	47.40	2.00	61.05	2.00	90.05	1.00
34.55	3.00	48.00	3.00	63.85	5.00	91.05	1.00
35.90	37.00	50.90	0.00	65.00	3.00	92.05	1.00

36.90	70.00	51.90	46.00	65.90	1.00	100.00	83.00
37.90	35.00	52.90	161.00	67.05	1.00	101.05	40.00
38.95	10.00	53.90	37.00	68.05	2.00	102.05	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
103.05	7.00	168.95	1.00				
106.05	5.00						
107.05	10.00						
108.05	9.00						
114.00	1.00						
120.05	2.00						
134.00	3.00						
134.20	1.00						
150.00	1.00						
150.20	1.00						
164.05	3.00						

#94: 5-METHYL-2-NITROBENZYL ALCOHOL
Modified: scaled

Entry Number 94 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 85.969
Mol Formula C8H9NO3
Mol Weight 167.057

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	92.00	38.90	3067.00	53.90	260.00	64.00	583.00
26.90	889.00	39.90	399.00	54.90	418.00	64.90	8026.00
28.90	459.00	40.90	1449.00	55.95	29.00	65.90	4081.00
29.90	473.00	41.90	141.00	57.00	21.00	66.90	847.00
30.90	314.00	46.90	123.00	57.90	0.00	67.90	98.00
32.95	2.00	47.85	11.00	58.10	6.00	68.90	47.00
33.85	2.00	48.90	58.00	58.90	41.00	69.95	17.00
35.15	0.00	49.90	892.00	59.90	24.00	71.05	10.00
35.90	4.00	50.90	2329.00	60.90	177.00	71.95	4.00
36.90	114.00	51.90	994.00	61.90	636.00	72.90	40.00
37.90	358.00	52.90	1529.00	62.90	1958.00	73.90	285.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
74.90	300.00	85.90	152.00	97.00	22.00	108.00	127.00
75.90	484.00	86.90	139.00	97.90	32.00	109.00	53.00
76.90	6608.00	88.05	58.00	99.00	14.00	110.05	8.00
77.95	4056.00	88.90	1642.00	99.90	2.00	111.05	8.00
79.00	1893.00	90.00	832.00	100.95	24.00	112.05	4.00
80.00	279.00	91.05	9437.00	101.95	205.00	113.05	2.00
81.00	266.00	92.05	2678.00	103.00	382.00	113.90	0.00

82.00	36.00	93.05	6509.00	104.05	9999.00	115.00	1.00
83.00	17.00	94.05	1389.00	105.00	1255.00	116.00	8.00
83.95	14.00	95.00	114.00	106.05	1041.00	117.05	19.00
84.90	57.00	96.00	14.00	107.05	812.00	118.00	633.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
119.00	2005.00	129.95	65.00	141.10	3.00	153.00	3.00
120.05	586.00	130.90	18.00	141.95	1.00	154.15	2.00
121.05	440.00	132.00	79.00	143.05	3.00	161.00	5.00
122.00	231.00	133.05	235.00	144.05	1.00	162.05	1.00
123.05	27.00	134.05	296.00	144.95	2.00	163.00	2.00
123.90	17.00	135.05	465.00	146.05	4.00	163.95	10.00
125.00	6.00	136.00	50.00	148.00	333.00	165.00	17.00
126.00	3.00	137.05	25.00	149.00	342.00	165.95	37.00
127.10	1.00	138.00	58.00	150.05	255.00	167.00	9.00
128.00	3.00	139.05	9.00	151.05	39.00	168.00	10.00
129.05	3.00	140.00	4.00	152.00	14.00	168.95	2.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
176.80	1.00						
178.00	2.00						
178.95	1.00						
180.00	1.00						
180.95	3.00						
182.05	4.00						
183.00	2.00						
192.95	1.00						
206.95	0.00						
208.95	1.00						

#95: 2-NITROTOLUENE
Modified: scaled

Entry Number 95 from C:\DATABASE\hjf.l
CAS 000088-72-2
Melting Point -300
Boiling Point -300
Retention Index 62.049
Mol Formula C7H7NO2
Mol Weight 137.048

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	69.00	40.95	486.00	53.95	17.00	67.05	36.00
26.90	226.00	42.00	23.00	55.00	19.00	68.05	10.00
27.90	22.00	42.90	64.00	56.00	3.00	71.90	4.00
28.90	59.00	45.90	37.00	58.95	1.00	73.00	29.00
29.90	218.00	46.90	2.00	60.00	18.00	74.05	157.00
30.90	8.00	47.95	6.00	60.90	159.00	75.05	140.00
36.00	6.00	48.90	48.00	61.95	479.00	76.05	140.00

36.90	134.00	49.90	608.00	63.05	1551.00	77.05	1655.00
37.90	334.00	50.90	1087.00	64.05	714.00	78.05	376.00
38.90	2277.00	52.05	345.00	65.05	7836.00	79.05	264.00
40.00	171.00	53.05	216.00	66.05	560.00	80.05	64.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
81.00	20.00	93.05	702.00	104.05	29.00	120.05	9999.00
82.05	4.00	94.05	37.00	105.05	28.00	121.05	833.00
83.05	0.00	95.05	1.00	106.05	47.00	122.05	52.00
83.90	5.00	97.05	0.00	107.05	56.00	123.05	4.00
85.05	50.00	98.00	2.00	108.05	13.00	128.10	1.00
86.00	97.00	98.30	0.00	109.05	3.00	129.05	0.00
87.00	74.00	99.05	5.00	110.10	1.00	130.15	1.00
89.05	1776.00	100.80	1.00	115.05	0.00	137.05	783.00
90.05	696.00	101.05	0.00	116.00	1.00	138.05	79.00
91.05	4296.00	102.05	10.00	117.10	3.00	139.05	7.00
92.05	4535.00	103.05	4.00	118.10	6.00	140.05	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
156.10	3.00						

#96: 4-METHYLNITROPHENOL
Modified: scaled

Entry Number 96 from C:\DATABASE\hjf.l
CAS 000106-44-5
Melting Point -300
Boiling Point -300
Retention Index 61.909
Mol Formula C7H8O
Mol Weight 108.057
Miscellaneous Information
Aldrich: p-cresol

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	114.00	36.90	85.00	47.95	6.00	59.00	0.00
26.90	589.00	37.90	197.00	48.90	67.00	59.95	10.00
27.90	4.00	38.95	825.00	49.90	461.00	60.95	71.00
28.90	97.00	39.90	133.00	50.90	841.00	62.00	150.00
29.95	3.00	40.95	56.00	52.05	442.00	63.00	339.00
30.90	13.00	41.90	37.00	53.05	842.00	64.05	82.00
32.80	0.00	42.95	98.00	54.00	435.00	65.05	177.00
33.40	0.00	44.95	12.00	54.90	232.00	66.05	102.00
34.65	0.00	45.90	3.00	55.95	9.00	67.00	41.00
35.00	1.00	46.75	1.00	57.05	3.00	68.05	42.00
35.95	6.00	47.05	0.00	58.00	0.00	69.95	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
71.95	3.00	83.05	1.00	94.00	3.00	110.05	41.00
73.00	25.00	83.95	6.00	95.40	0.00	111.05	2.00

74.05	87.00	85.00	18.00	99.15	0.00	112.05	0.00
75.05	42.00	86.00	27.00	100.95	2.00	115.10	0.00
76.05	0.00	87.05	20.00	102.00	0.00	116.10	0.00
77.05	2356.00	88.00	5.00	103.05	2.00	121.15	0.00
78.05	481.00	89.05	266.00	104.05	0.00	128.15	0.00
79.05	1909.00	90.05	937.00	105.05	81.00	133.05	0.00
80.05	906.00	91.05	407.00	107.05	9999.00	144.20	0.00
81.05	153.00	92.05	36.00	108.05	9343.00	152.15	2.00
82.05	22.00	93.05	16.00	109.05	717.00	165.10	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
166.20	0.00						
167.15	2.00						
183.15	0.00						

#97: 2-NITRO-1,3-DIMETHYLBENZENE
Modified: scaled

Entry Number 97 from C:\DATABASE\hjf.l
CAS 000081-20-9
Melting Point -300
Boiling Point -300
Retention Index 62.71
Mol Formula C8H9NO2
Mol Weight 151.062
Miscellaneous Information
Aldrich: 2-nitro-m-xylene

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	73.00	39.90	167.00	55.00	58.00	64.00	296.00
26.90	1011.00	41.00	363.00	56.00	7.00	65.00	1141.00
28.90	103.00	42.00	34.00	56.95	1.00	66.05	303.00
29.90	219.00	46.95	5.00	57.30	1.00	67.00	281.00
30.90	24.00	48.00	5.00	57.55	1.00	68.00	37.00
33.05	1.00	48.95	39.00	57.80	2.00	70.05	4.00
33.85	1.00	49.90	636.00	58.55	6.00	71.95	2.00
35.90	3.00	50.90	1762.00	59.95	16.00	72.95	33.00
36.90	83.00	51.95	615.00	60.90	105.00	73.95	222.00
37.90	246.00	53.05	915.00	61.95	348.00	74.95	215.00
38.90	1841.00	54.00	81.00	62.95	1042.00	76.05	314.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
77.05	7881.00	88.05	24.00	99.00	13.00	115.05	3.00
78.05	2313.00	89.05	535.00	100.00	1.00	116.05	124.00
79.05	9999.00	90.05	150.00	101.05	48.00	117.05	34.00
80.05	733.00	91.05	1277.00	102.05	438.00	118.05	46.00
81.05	81.00	92.05	271.00	103.05	3124.00	119.05	47.00
82.00	16.00	93.05	145.00	104.05	1242.00	120.05	25.00
83.05	5.00	94.05	62.00	105.05	2061.00	121.05	94.00

83.95	5.00	95.05	11.00	106.05	4235.00	122.05	22.00
85.00	28.00	96.05	4.00	107.05	642.00	123.05	2.00
86.00	61.00	97.00	8.00	110.05	1.00	130.10	3.00
87.05	69.00	98.00	32.00	113.95	1.00	132.05	89.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
134.05	9901.00						
135.05	907.00						
136.05	62.00						
137.05	4.00						
148.00	4.00						
151.05	3660.00						
152.05	349.00						
153.05	30.00						
154.10	3.00						

#98: 4,6-DIMETHYL-2H-PYRAN-2-ONE
Modified: scaled

Entry Number 98 from C:\DATABASE\hjf.l
CAS 000675-09-2
Melting Point -300
Boiling Point -300
Retention Index 69.549
Mol Formula C7H8O2
Mol Weight 124.052
Miscellaneous Information
Aldrich: 4,6-dimethyl-alpha-pyrone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	266.00	40.00	350.00	54.05	442.00	66.00	357.00
26.90	1797.00	40.90	757.00	54.90	103.00	67.05	2746.00
28.90	57.00	41.95	355.00	55.95	71.00	68.05	1624.00
29.95	3.00	43.00	4401.00	57.00	9.00	68.90	216.00
30.95	18.00	46.95	44.00	58.10	3.00	69.90	9.00
33.65	3.00	47.95	35.00	59.95	18.00	70.95	3.00
34.60	2.00	48.90	152.00	60.90	85.00	72.05	5.00
35.90	17.00	49.90	836.00	61.90	128.00	72.95	23.00
36.90	264.00	50.90	1194.00	62.95	162.00	73.95	60.00
37.90	683.00	52.05	704.00	64.05	36.00	74.95	18.00
38.90	1606.00	53.05	7554.00	65.05	342.00	76.00	10.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
77.05	120.00	92.05	3.00	111.00	19.00	141.20	2.00
78.00	44.00	92.95	33.00	112.05	1.00	142.10	4.00
79.05	106.00	95.05	3003.00	115.05	1.00	150.00	1.00
80.00	11.00	96.05	9999.00	120.05	1.00	163.95	1.00
81.05	1763.00	97.05	625.00	122.15	1.00		
82.05	263.00	98.05	39.00	124.05	7908.00		

83.05	18.00	99.05	2.00	125.05	702.00
83.95	5.00	106.05	5.00	126.05	59.00
85.00	11.00	107.05	1.00	127.10	6.00
88.90	1.00	109.05	2954.00	132.05	2.00
91.00	2.00	110.05	189.00	134.95	1.00

#99: 3,4-DIMETHYL-2,5-FURANDIONE
Modified: scaled

Entry Number 99 from C:\DATABASE\hjf.l
CAS 000766-39-2
Melting Point -300
Boiling Point -300
Retention Index 58.649
Mol Formula C6H6O3
Mol Weight 126.03
Miscellaneous Information
Aldrich: 2,3-dimethylmaleic anhydride

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	917.00	38.90	8937.00	54.05	9999.00	67.00	268.00
26.90	2668.00	40.00	368.00	55.05	550.00	68.05	18.00
27.90	1636.00	42.00	106.00	56.05	20.00	68.90	45.00
28.90	129.00	44.90	30.00	57.00	4.00	70.00	80.00
30.00	0.00	46.90	1.00	59.90	12.00	70.95	7.00
30.95	4.00	47.90	60.00	60.95	21.00	71.90	1.00
32.95	2.00	48.90	386.00	61.95	16.00	72.10	2.00
34.00	1.00	49.90	1309.00	63.00	8.00	76.00	1.00
35.90	77.00	50.90	1355.00	63.95	5.00	76.90	9.00
36.90	492.00	52.05	894.00	64.95	18.00	78.05	2.00
38.00	633.00	53.05	3203.00	65.95	101.00	78.95	6.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
80.00	27.00	102.15	1.00				
82.05	5612.00	110.05	7.00				
83.05	302.00	124.10	4.00				
84.05	22.00	126.05	3688.00				
85.00	4.00	127.05	320.00				
91.10	2.00	128.05	35.00				
93.15	1.00	129.05	2.00				
97.00	12.00	181.00	0.00				
98.00	11.00						
99.05	3.00						
101.05	1.00						

#100: trans, trans-2,4-NONADIENAL
Modified: scaled

Entry Number 100 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 64.95
Mol Formula C9H14O
Mol Weight 138.104

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	59.00	37.95	74.00	52.05	130.00	63.00	79.00
26.90	926.00	38.90	1278.00	53.05	832.00	64.00	20.00
27.90	20.00	40.00	266.00	54.05	716.00	65.05	487.00
28.90	426.00	41.00	2176.00	55.05	690.00	66.05	368.00
29.95	8.00	42.05	143.00	56.05	325.00	67.05	1360.00
30.90	40.00	43.05	546.00	57.05	61.00	68.05	512.00
32.90	1.00	46.85	1.00	58.05	2.00	69.00	121.00
33.15	0.00	47.85	1.00	59.00	4.00	70.05	118.00
33.60	1.00	48.95	6.00	60.00	11.00	71.05	12.00
35.90	1.00	49.90	104.00	60.90	9.00	72.00	2.00
36.90	19.00	50.90	269.00	61.90	27.00	72.95	3.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
73.95	14.00	86.05	3.00	97.05	20.00	109.05	192.00
75.00	9.00	87.00	2.00	98.00	2.00	110.05	25.00
76.05	3.00	88.05	1.00	99.00	1.00	111.10	3.00
77.05	366.00	89.00	6.00	101.05	1.00	115.05	3.00
78.05	108.00	90.05	1.00	102.05	2.00	116.05	1.00
79.05	601.00	91.05	149.00	103.05	9.00	117.05	3.00
81.05	9999.00	92.05	29.00	104.05	3.00	118.05	2.00
82.05	924.00	93.05	38.00	105.05	37.00	119.00	4.00
83.05	738.00	94.05	116.00	106.05	5.00	120.05	11.00
84.05	58.00	95.05	665.00	107.05	41.00	121.05	7.00
85.00	6.00	96.05	132.00	108.10	9.00	122.10	3.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
123.05	31.00	140.15	9.00				
124.05	3.00	141.15	1.00				
130.05	1.00	163.95	0.00				
132.05	0.00						
133.10	1.00						
134.05	0.00						
135.05	1.00						
136.10	4.00						
137.10	70.00						
138.20	941.00						
139.20	118.00						

#101: 4-METHYLMORPHOLINE

Modified: scaled

Entry Number 101 from C:\DATABASE\hjf.l
CAS 000109-02-4
Melting Point -300
Boiling Point -300
Retention Index 25.769
Mol Formula C5H11NO
Mol Weight 101.084

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	146.00	39.05	55.00	50.90	25.00	65.55	19.00
27.90	715.00	39.90	76.00	52.05	46.00	65.90	20.00
28.90	356.00	40.90	457.00	52.90	35.00	67.15	21.00
29.90	181.00	41.90	3886.00	54.05	153.00	68.05	50.00
30.90	74.00	43.05	9999.00	55.05	110.00	68.90	10.00
33.90	22.00	43.90	1454.00	56.05	457.00	70.05	425.00
35.40	18.00	44.90	15.00	56.90	107.00	71.05	2401.00
36.15	16.00	45.90	63.00	58.05	134.00	72.05	242.00
36.65	19.00	46.85	6.00	59.05	24.00	73.05	44.00
37.30	15.00	48.30	28.00	59.95	10.00	78.05	20.00
37.85	29.00	49.60	26.00	65.05	19.00	80.90	24.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
82.05	25.00	103.05	26.00				
83.05	21.00	118.90	3.00				
83.90	36.00	150.05	20.00				
85.05	26.00						
86.05	59.00						
97.15	21.00						
98.05	41.00						
99.05	102.00						
100.00	1489.00						
101.05	4350.00						
102.05	274.00						

#102: 5-METHYL-5-HEXEN-2-ONE
Modified: scaled

Entry Number 102 from C:\DATABASE\hjf.l
CAS 003240-09-3
Melting Point -300
Boiling Point -300
Retention Index 37.039
Mol Formula C7H12O
Mol Weight 112.088

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.

25.95	78.00	35.85	2.00	48.65	18.00	60.00	2.00
26.90	728.00	36.85	37.00	49.90	92.00	60.90	10.00
27.90	46.00	37.90	103.00	50.90	154.00	62.05	21.00
28.90	451.00	38.90	1230.00	52.00	61.00	63.05	30.00
29.95	11.00	40.00	212.00	53.00	457.00	64.05	5.00
30.90	26.00	41.00	3866.00	54.05	102.00	65.00	68.00
32.90	5.00	42.05	424.00	55.05	1217.00	66.00	26.00
33.75	2.00	42.90	9999.00	56.00	84.00	67.05	397.00
34.05	1.00	44.90	16.00	57.05	68.00	68.05	309.00
34.80	0.00	46.95	1.00	58.00	89.00	69.00	3590.00
35.15	0.00	47.55	2.00	59.05	24.00	70.05	1078.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
71.05	266.00	82.05	10.00	93.00	26.00	112.00	499.00
72.05	14.00	83.05	46.00	94.05	62.00	113.05	52.00
73.05	3.00	84.00	6.00	95.05	65.00	114.00	3.00
74.00	5.00	85.05	10.00	97.05	2715.00	122.15	0.00
74.95	2.00	85.95	1.00	98.05	184.00	123.15	0.00
75.95	0.00	87.10	1.00	99.05	11.00	137.10	1.00
77.05	108.00	88.90	0.00	107.05	2.00	164.05	0.00
78.00	13.00	89.15	0.00	108.05	0.00		
79.05	219.00	89.90	0.00	109.05	5.00		
80.05	17.00	91.05	30.00	110.10	3.00		
81.05	28.00	92.05	4.00	111.05	34.00		

#103: BENZENEMETHANOL
Modified: scaled

Entry Number 103 from C:\DATABASE\hjf.l
CAS 000100-51-6
Melting Point -300
Boiling Point -300
Retention Index 55.079
Mol Formula C7H8O
Mol Weight 108.057
Miscellaneous Information
Aldrich: benzyl alcohol

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	80.00	38.90	993.00	55.95	4.00	67.95	12.00
26.95	444.00	39.90	93.00	56.95	1.00	70.30	1.00
28.90	285.00	40.95	75.00	58.95	1.00	70.90	0.00
29.95	24.00	42.00	20.00	59.95	13.00	71.95	5.00
30.90	224.00	47.95	9.00	60.95	93.00	72.95	63.00
32.90	1.00	48.90	87.00	61.95	219.00	74.00	267.00
34.15	1.00	49.90	905.00	63.00	530.00	75.00	139.00
34.40	0.00	50.90	2012.00	64.05	130.00	76.05	162.00
35.85	9.00	52.05	589.00	65.05	703.00	77.05	5296.00

36.90	126.00	53.00	678.00	66.05	70.00	78.05	1121.00
37.90	258.00	54.95	59.00	67.05	10.00	79.05	9999.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
80.05	938.00	91.05	1433.00	107.05	5911.00		
81.05	55.00	92.05	123.00	108.05	9057.00		
82.00	5.00	93.00	6.00	109.05	687.00		
82.65	0.00	93.95	2.00	110.05	40.00		
83.95	9.00	94.90	1.00	111.05	3.00		
85.00	31.00	96.05	0.00	128.10	2.00		
86.00	48.00	100.95	2.00	149.95	0.00		
87.00	31.00	101.90	0.00	155.10	5.00		
88.05	3.00	103.05	4.00	219.95	0.00		
89.05	673.00	105.05	443.00				
90.05	777.00	106.05	192.00				

#104: 5-NITRO-M-XYLENE
Modified: scaled

Entry Number 104 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 72.549
Mol Formula C8H9NO2
Mol Weight 151.062
Miscellaneous Information
Aldrich (1,3-dimethyl-5-nitro-benzene)

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	45.00	41.00	241.00	55.05	60.00	67.05	56.00
26.90	881.00	41.95	15.00	56.00	5.00	68.05	9.00
28.95	69.00	45.90	23.00	57.05	1.00	70.00	0.00
29.90	256.00	46.95	0.00	58.50	3.00	71.05	2.00
33.05	0.00	47.90	4.00	59.85	6.00	72.00	3.00
33.90	0.00	48.95	31.00	60.90	85.00	73.00	26.00
35.95	3.00	49.90	462.00	61.95	321.00	74.00	184.00
36.90	64.00	50.95	1222.00	63.05	1021.00	75.00	165.00
37.90	229.00	52.05	377.00	64.00	260.00	76.05	206.00
38.90	1626.00	53.05	751.00	65.00	782.00	77.05	6017.00
39.95	142.00	54.05	49.00	66.05	110.00	78.05	1364.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
79.05	6521.00	90.05	96.00	101.00	37.00	116.05	7.00
80.05	439.00	91.05	835.00	102.05	318.00	117.05	8.00
81.00	20.00	92.05	89.00	103.05	3741.00	118.05	19.00
82.00	3.00	93.05	508.00	104.05	942.00	119.05	13.00
83.00	2.00	94.05	62.00	105.05	9383.00	120.10	7.00
83.95	3.00	95.05	9.00	106.05	830.00	121.05	1300.00

85.00	24.00	96.00	3.00	107.05	35.00	122.05	112.00
86.00	66.00	96.95	7.00	108.05	6.00	123.05	8.00
87.05	68.00	98.00	35.00	109.05	8.00	129.15	1.00
88.00	18.00	99.05	10.00	110.00	1.00	132.00	2.00
89.05	321.00	100.00	1.00	110.90	0.00	133.15	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
134.05	99.00	154.10	5.00				
135.05	135.00	164.05	0.00				
136.05	25.00	181.05	1.00				
137.10	4.00	182.15	1.00				
144.05	0.00	195.20	0.00				
145.20	1.00	210.10	1.00				
147.10	2.00	211.05	1.00				
149.05	22.00	212.20	5.00				
151.05	9999.00	220.05	1.00				
152.05	991.00						
153.05	82.00						

#105: 2,6-DINITRO-4-METHYLPHENOL
Modified: scaled

Entry Number 105 from C:\DATABASE\hjf.l
CAS 000609-93-8
Melting Point -300
Boiling Point -300
Retention Index 88.78
Mol Formula C7H6N2O5
Mol Weight 198.027
Miscellaneous Information
Aldrich: 2,6-dinitro-p-cresol

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	115.00	40.00	505.00	52.05	2620.00	63.05	784.00
26.90	685.00	41.00	486.00	52.90	2917.00	64.05	629.00
28.90	142.00	42.00	122.00	54.05	424.00	65.05	3158.00
29.90	1921.00	43.05	1017.00	55.00	291.00	66.05	1850.00
30.90	8.00	44.90	69.00	56.05	65.00	67.00	373.00
33.55	1.00	45.90	46.00	57.05	31.00	68.05	165.00
34.90	2.00	46.90	6.00	58.00	5.00	69.00	256.00
35.85	14.00	47.95	13.00	59.00	1.00	70.05	103.00
36.90	230.00	48.95	102.00	59.95	15.00	71.05	23.00
37.90	424.00	49.90	1616.00	60.90	182.00	72.00	9.00
38.90	2440.00	50.95	5280.00	61.95	461.00	72.95	64.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
74.00	392.00	85.05	33.00	96.05	77.00	107.05	868.00
75.05	396.00	85.95	48.00	97.05	273.00	108.05	79.00
76.05	847.00	87.00	49.00	98.05	25.00	109.05	56.00

77.05	4349.00	88.00	30.00	99.05	7.00	110.05	300.00
78.05	1034.00	89.05	33.00	100.05	1.00	111.05	27.00
79.05	421.00	90.05	90.00	101.00	10.00	112.05	29.00
80.05	139.00	91.05	366.00	102.00	13.00	113.10	5.00
81.05	149.00	92.05	218.00	103.05	30.00	114.00	0.00
82.05	746.00	93.05	841.00	104.05	207.00	115.05	2.00
83.05	78.00	94.05	457.00	105.05	1576.00	116.05	4.00
84.05	62.00	95.05	164.00	106.05	919.00	117.05	4.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
118.05	12.00	129.05	4.00	142.05	36.00	154.05	5.00
119.00	14.00	130.05	4.00	143.05	5.00	155.10	5.00
120.05	104.00	132.00	10.00	145.05	5.00	158.05	2.00
121.05	1157.00	133.05	9.00	146.05	5.00	159.05	1.00
122.05	466.00	134.05	45.00	147.05	4.00	161.00	3.00
123.05	690.00	135.05	881.00	148.10	6.00	161.20	2.00
124.05	82.00	136.05	83.00	149.05	7.00	162.05	6.00
125.05	13.00	137.05	60.00	150.05	47.00	163.10	5.00
126.05	4.00	138.05	61.00	151.05	767.00	164.00	2.00
127.10	2.00	140.05	4454.00	152.05	109.00	165.05	74.00
128.05	4.00	141.05	316.00	153.05	25.00	166.05	16.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
167.15	11.00	183.05	21.00	200.05	147.00		
168.05	1414.00	184.05	9.00	201.05	10.00		
169.05	119.00	191.10	3.00	207.05	2.00		
170.05	19.00	192.05	7.00	208.05	1.00		
176.00	1.00	193.00	7.00	209.00	3.00		
177.05	5.00	194.05	4.00	211.20	2.00		
178.05	9.00	195.20	2.00	220.10	4.00		
179.05	5.00	196.05	45.00				
180.05	12.00	197.05	27.00				
181.00	23.00	198.05	9999.00				
182.05	215.00	199.05	892.00				

#106: 2,5-DIHYDRO-2,5-DIMETHOXYFURAN
Modified: scaled

Entry Number 106 from C:\DATABASE\hjf.l
CAS 000332-77-4
Melting Point -300
Boiling Point -300
Retention Index 38.82
Mol Formula C6H10O3
Mol Weight 130.062

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	152.00	35.80	4.00	47.80	3.00	58.90	507.00
27.00	821.00	36.05	13.00	48.55	4.00	59.90	32.00

27.90	130.00	36.95	54.00	48.95	2.00	60.95	19.00
28.90	1045.00	37.95	158.00	50.00	7.00	63.05	4.00
29.90	90.00	38.90	897.00	51.05	10.00	63.40	4.00
30.90	210.00	39.90	320.00	52.10	16.00	63.80	4.00
31.90	31.00	40.95	2492.00	52.95	144.00	66.00	17.00
32.90	45.00	42.05	557.00	53.95	53.00	67.00	50.00
33.75	7.00	44.90	397.00	54.90	721.00	68.05	240.00
33.95	4.00	45.90	12.00	56.00	262.00	68.90	475.00
34.80	6.00	47.00	21.00	56.95	26.00	70.05	227.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
71.05	3107.00	85.00	31.00	102.05	47.00		
72.05	136.00	86.05	19.00	113.05	4.00		
73.00	20.00	87.05	26.00	113.95	4.00		
73.90	10.00	88.05	17.00	115.05	30.00		
75.05	50.00	91.05	4.00	129.05	518.00		
75.80	4.00	95.05	3.00	130.05	58.00		
81.00	7.00	97.10	8.00	163.95	4.00		
81.30	3.00	98.05	200.00				
82.05	13.00	99.05	9999.00				
82.95	265.00	100.05	609.00				
84.00	71.00	101.05	578.00				

#107: 5-METHYL-2-NITROPHENOL
Modified: scaled

Entry Number 107 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 68.299
Mol Formula C7H7NO3
Mol Weight 153.042

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.15	8.00	38.90	1805.00	52.90	1793.00	65.05	1694.00
26.00	91.00	39.90	194.00	53.95	157.00	66.05	501.00
27.05	813.00	41.05	466.00	54.95	933.00	67.00	1210.00
28.90	130.00	41.95	74.00	56.00	71.00	68.05	112.00
29.90	361.00	44.90	9.00	57.05	136.00	68.90	34.00
31.00	63.00	47.00	10.00	58.00	12.00	70.00	35.00
34.00	3.00	47.80	9.00	59.95	28.00	71.05	94.00
34.85	13.00	48.90	83.00	60.90	109.00	71.95	19.00
35.95	7.00	49.90	850.00	61.90	307.00	72.95	33.00
36.95	148.00	50.95	1933.00	63.00	842.00	73.95	184.00
37.90	454.00	52.00	1560.00	64.05	269.00	75.00	107.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
76.05	277.00	86.95	40.00	98.10	20.00	119.00	19.00

77.05	5107.00	88.00	19.00	99.05	28.00	120.05	335.00
78.05	1985.00	89.05	65.00	100.95	12.00	121.05	55.00
79.05	795.00	90.00	56.00	103.05	6.00	122.05	70.00
80.00	96.00	91.00	102.00	104.10	25.00	123.05	2339.00
81.00	91.00	92.05	247.00	105.05	614.00	124.05	190.00
82.05	36.00	93.05	45.00	106.05	219.00	125.10	28.00
83.05	24.00	94.05	119.00	107.05	507.00	126.10	12.00
84.00	12.00	95.05	1440.00	108.05	200.00	131.00	2.00
85.05	55.00	96.05	100.00	109.10	39.00	133.05	12.00
85.95	30.00	97.05	37.00	112.00	21.00	136.05	333.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
137.05	149.00						
138.05	24.00						
141.10	12.00						
150.00	1.00						
153.05	9999.00						
154.05	819.00						
155.05	100.00						
181.05	7.00						

#108: 2-FURALDEHYDE
Modified: scaled

Entry Number 108 from C:\DATABASE\hjf.l
CAS 000098-01-1
Melting Point -300
Boiling Point -300
Retention Index 36.49
Mol Formula C5H4O2
Mol Weight 96.021

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	136.00	41.90	374.00	55.95	3.00	68.90	37.00
26.90	52.00	43.05	15.00	58.00	0.00	69.90	9.00
28.90	1133.00	46.65	0.00	59.90	7.00	71.90	0.00
29.90	15.00	47.85	37.00	60.90	13.00	72.10	0.00
33.90	77.00	48.90	116.00	61.95	6.00	74.15	0.00
35.90	113.00	49.90	207.00	62.95	2.00	76.00	1.00
36.90	762.00	50.90	287.00	63.90	5.00	77.00	5.00
37.90	1450.00	51.90	48.00	64.90	19.00	78.05	0.00
38.90	4407.00	52.90	141.00	65.90	93.00	79.00	6.00
39.90	453.00	53.90	10.00	66.95	1136.00	80.05	7.00
40.90	151.00	55.00	2.00	68.00	138.00	81.00	2.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
82.05	0.00	134.05	1.00				
83.00	0.00						
92.00	1.00						

93.00	6.00
95.05	9140.00
96.05	9999.00
97.00	642.00
98.00	58.00
99.00	4.00
112.10	0.00
113.05	0.00

#109: 5-(HYDROXYMETHYL)FURFURAL
Modified: scaled

Entry Number 109 from C:\DATABASE\hjf.l
CAS 000067-47-0
Melting Point -300
Boiling Point -300
Retention Index 76.859
Mol Formula C6H6O3
Mol Weight 126.031

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	242.00	34.60	3.00	45.80	4.00	54.95	184.00
26.95	549.00	35.00	20.00	46.05	5.00	55.65	3.00
27.90	372.00	35.95	60.00	46.30	4.00	55.95	24.00
28.90	1263.00	36.90	454.00	46.65	3.00	57.05	5.00
29.95	77.00	37.90	933.00	47.95	25.00	57.15	5.00
30.95	609.00	38.90	3304.00	48.90	144.00	57.30	3.00
31.90	11.00	39.90	319.00	49.90	619.00	57.80	4.00
32.80	10.00	41.00	6112.00	50.90	1079.00	57.90	17.00
32.90	5.00	41.95	559.00	51.95	598.00	58.05	13.00
33.05	5.00	42.95	281.00	52.95	1399.00	60.00	19.00
33.95	45.00	44.90	16.00	54.00	132.00	60.90	39.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
61.95	49.00	70.95	45.00	91.80	3.00	110.05	292.00
62.85	20.00	73.05	3.00	93.00	41.00	111.05	34.00
63.05	7.00	73.80	3.00	94.05	43.00	112.15	3.00
63.85	17.00	77.00	31.00	95.05	458.00	118.95	2.00
64.05	8.00	78.00	15.00	96.05	31.00	123.05	629.00
64.95	60.00	79.00	194.00	97.00	9999.00	124.05	730.00
66.00	190.00	80.05	228.00	98.05	584.00	125.05	809.00
66.95	279.00	81.05	496.00	99.05	68.00	126.05	4997.00
68.00	282.00	82.00	49.00	100.00	6.00	127.05	364.00
68.95	3069.00	85.95	7.00	108.05	30.00	128.05	52.00
69.95	180.00	91.05	3.00	109.05	816.00	131.00	4.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
168.95	1.00						
218.95	6.00						

#110: 2,5-DIMETHYLBENZALDEHYDE
Modified: scaled

Entry Number 110 from C:\DATABASE\hjf.l
CAS 005779-94-2
Melting Point -300
Boiling Point -300
Retention Index 61.549
Mol Formula C9H10O
Mol Weight 134.073

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	43.00	39.90	92.00	54.00	33.00	65.05	621.00
26.90	573.00	40.95	129.00	55.05	43.00	66.05	247.00
28.90	125.00	42.00	9.00	56.05	7.00	67.00	152.00
29.95	2.00	43.05	50.00	57.05	19.00	70.05	4.00
34.80	0.00	44.95	15.00	59.00	39.00	71.05	1.00
35.05	1.00	48.00	1.00	59.65	3.00	71.90	2.00
35.30	0.00	48.90	29.00	59.90	2.00	73.00	26.00
36.05	2.00	49.90	459.00	60.90	67.00	73.95	175.00
36.90	47.00	50.95	1273.00	61.95	211.00	75.00	146.00
37.95	131.00	52.00	330.00	63.00	590.00	76.05	158.00
38.90	1010.00	53.05	448.00	64.05	124.00	77.05	2537.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
78.05	797.00	90.05	85.00	103.05	1609.00	115.05	50.00
79.05	2323.00	91.05	2278.00	104.05	440.00	116.05	10.00
80.05	151.00	92.05	170.00	105.05	8444.00	117.05	7.00
81.00	6.00	93.05	7.00	106.05	948.00	118.05	18.00
82.05	1.00	94.05	3.00	107.05	60.00	119.05	209.00
83.05	4.00	96.10	2.00	108.05	4.00	120.05	19.00
85.00	23.00	97.05	10.00	109.00	2.00	121.05	2.00
86.00	44.00	98.05	33.00	110.10	3.00	125.10	1.00
87.05	48.00	99.05	9.00	111.10	3.00	129.05	3.00
88.00	13.00	101.05	32.00	113.05	4.00	130.10	2.00
89.05	256.00	102.05	221.00	114.00	1.00	131.05	16.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
133.05	9455.00	211.20	5.00				
134.05	9999.00	239.20	2.00				
135.05	974.00						
136.10	60.00						
137.05	4.00						
142.00	1.00						
164.05	0.00						
167.20	0.00						
168.10	2.00						
180.95	0.00						

183.20 2.00

#111: 4-ETHYLBENZALDEHYDE
Modified: scaled

Entry Number 111 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 62.439
Mol Formula C9H10O
Mol Weight 134.073

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	50.00	41.95	5.00	56.00	2.00	66.95	1.00
26.90	591.00	43.05	27.00	57.00	1.00	68.15	1.00
28.90	204.00	44.90	17.00	57.80	2.00	70.10	1.00
29.95	2.00	47.90	2.00	58.95	10.00	72.00	1.00
33.00	0.00	48.90	38.00	59.90	5.00	73.00	44.00
35.90	2.00	49.90	629.00	60.90	73.00	74.00	273.00
36.90	57.00	50.95	1495.00	61.95	232.00	75.00	221.00
37.90	155.00	51.95	267.00	63.00	690.00	76.05	268.00
38.90	948.00	53.05	247.00	64.05	170.00	77.05	2529.00
39.95	79.00	53.95	16.00	65.05	887.00	78.05	647.00
40.95	136.00	55.00	24.00	66.05	135.00	79.05	2414.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
80.05	149.00	93.05	11.00	106.05	564.00	119.05	1426.00
81.05	4.00	94.00	2.00	107.05	56.00	120.05	108.00
83.15	0.00	95.05	1.00	108.05	3.00	121.05	6.00
85.05	22.00	97.05	6.00	108.95	2.00	128.10	1.00
86.00	46.00	98.00	34.00	110.05	2.00	129.05	5.00
87.05	50.00	99.05	10.00	111.00	0.00	131.05	77.00
88.00	18.00	101.05	46.00	113.05	2.00	133.05	9934.00
89.05	681.00	102.05	224.00	115.05	30.00	134.05	9999.00
90.05	417.00	103.05	1570.00	116.05	10.00	135.05	1000.00
91.05	4299.00	104.05	321.00	117.00	17.00	136.10	62.00
92.05	325.00	105.05	5318.00	118.05	74.00	137.05	2.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
142.20	0.00						
154.20	1.00						
155.10	10.00						
156.10	2.00						
167.05	0.00						
181.10	1.00						
183.20	5.00						
211.20	2.00						
239.20	0.00						

#112: 4-HYDROXY-3-METHYLBENZALDEHYDE
Modified: scaled

Entry Number 112 from C:\DATABASE\hjf.l
CAS 015174-69-3
Melting Point -300
Boiling Point -300
Retention Index 85.799
Mol Formula C8H8O2
Mol Weight 136.051

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	57.00	39.90	61.00	53.95	184.00	66.05	61.00
26.90	386.00	41.05	46.00	54.95	148.00	67.05	164.00
28.90	163.00	42.00	21.00	56.05	10.00	67.90	17.00
29.95	5.00	43.00	97.00	57.05	5.00	70.05	9.00
30.95	7.00	45.90	0.00	58.45	17.00	71.05	2.00
33.05	1.00	47.90	5.00	59.90	8.00	72.05	2.00
35.00	1.00	48.95	47.00	60.90	61.00	73.00	32.00
35.90	5.00	49.90	409.00	62.05	142.00	74.05	137.00
36.90	82.00	50.95	821.00	63.05	353.00	75.05	72.00
37.90	178.00	52.05	419.00	64.05	78.00	76.05	67.00
38.90	785.00	53.05	641.00	65.05	90.00	77.05	2575.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
78.05	488.00	89.05	166.00	101.00	2.00	115.00	0.00
79.05	1480.00	90.05	113.00	102.00	1.00	116.05	1.00
80.05	122.00	91.05	55.00	103.05	2.00	117.05	38.00
81.05	30.00	92.05	15.00	105.05	111.00	118.05	8.00
82.05	24.00	93.05	12.00	106.05	188.00	119.05	4.00
83.05	28.00	94.05	3.00	107.05	3149.00	120.05	2.00
84.05	5.00	95.05	3.00	108.05	309.00	121.05	3.00
85.05	16.00	96.05	3.00	109.05	20.00	122.05	0.00
86.05	26.00	97.05	12.00	110.05	2.00	123.05	1.00
87.05	24.00	98.05	3.00	111.15	5.00	124.10	1.00
88.05	8.00	99.10	1.00	112.10	1.00	125.10	3.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
126.10	1.00	144.20	1.00	166.05	4.00	191.20	1.00
127.15	1.00	145.15	2.00	167.05	22.00	192.25	2.00
128.05	0.00	147.05	1.00	168.05	2.00	195.20	1.00
132.30	1.00	149.05	10.00	169.05	0.00	196.20	2.00
133.05	23.00	150.10	1.00	170.20	2.00	197.20	3.00
135.05	9999.00	151.05	1.00	175.20	1.00	198.20	1.00
136.05	8115.00	152.05	2.00	181.05	1.00	207.05	1.00
137.05	860.00	153.10	1.00	182.20	2.00	209.20	1.00
138.05	72.00	154.10	1.00	183.20	1.00	210.20	2.00
139.15	6.00	155.15	1.00	185.20	2.00	215.20	2.00

140.15	0.00	161.15	3.00	187.20	1.00	220.15	3.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
224.30	2.00						
225.20	1.00						

#113: 2-HYDROXY-5-NITROBENZALDEHYDE
Modified: scaled

Entry Number 113 from C:\DATABASE\hjf.l
CAS 000097-51-8
Melting Point -300
Boiling Point -300
Retention Index 83.659
Mol Formula C7H5NO4
Mol Weight 167.021

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	121.00	39.90	130.00	52.90	1958.00	65.05	3949.00
27.00	240.00	41.00	60.00	54.00	173.00	66.05	427.00
27.90	86.00	42.00	76.00	55.05	487.00	67.05	140.00
28.90	406.00	43.05	71.00	56.05	14.00	68.05	61.00
29.90	311.00	44.90	7.00	58.00	3.00	68.90	74.00
30.95	32.00	45.95	72.00	58.95	5.00	70.05	22.00
33.85	3.00	47.90	7.00	59.90	54.00	72.05	2.00
35.90	26.00	48.90	80.00	60.90	309.00	72.95	88.00
36.90	252.00	49.95	437.00	61.95	684.00	74.05	420.00
37.90	576.00	50.90	489.00	63.05	1487.00	75.05	1213.00
38.90	3115.00	52.00	323.00	64.05	761.00	76.05	151.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
77.05	56.00	89.00	26.00	100.95	12.00	112.10	7.00
78.05	37.00	90.05	59.00	102.05	3.00	115.00	12.00
79.05	136.00	91.00	228.00	103.05	606.00	117.10	7.00
80.05	194.00	92.05	872.00	104.05	61.00	118.10	11.00
81.05	632.00	93.00	1466.00	105.05	16.00	119.00	47.00
82.05	61.00	94.05	114.00	106.05	16.00	120.05	1850.00
83.05	24.00	95.05	22.00	107.05	99.00	121.05	691.00
84.00	0.00	96.05	32.00	108.05	254.00	122.05	72.00
85.90	4.00	97.05	17.00	109.05	571.00	123.05	16.00
87.00	14.00	98.10	4.00	110.05	43.00	124.15	11.00
87.95	9.00	100.00	2.00	111.10	7.00	125.10	5.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
126.10	4.00	140.15	4.00	163.10	16.00	219.95	3.00
128.15	3.00	141.20	1.00	164.00	7.00		
131.05	2.00	145.10	0.00	166.05	2259.00		
132.00	9.00	147.20	7.00	167.05	9999.00		
133.05	10.00	148.20	3.00	168.05	876.00		
134.15	10.00	149.05	281.00	169.05	113.00		

135.05	73.00	150.05	34.00	170.05	14.00
136.05	149.00	151.05	381.00	178.20	7.00
137.05	2254.00	152.05	47.00	181.05	8.00
138.05	203.00	153.05	18.00	182.20	8.00
139.05	74.00	155.15	9.00	207.05	4.00

#114: ALPHA-METHYLBENZENEACETALDEHYDE
Modified: scaled

Entry Number 114 from C:\DATABASE\hjf.l
CAS 000093-53-8
Melting Point -300
Boiling Point -300
Retention Index 56.5
Mol Formula C9H10O
Mol Weight 134.073
Miscellaneous Information
Aldrich: 2-phenylpropionaldehyde

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	25.00	38.90	385.00	51.90	156.00	64.00	51.00
26.90	311.00	39.90	30.00	52.95	110.00	65.00	224.00
27.90	14.00	41.00	36.00	54.00	7.00	66.05	28.00
28.90	99.00	41.90	2.00	55.00	14.00	66.90	2.00
30.00	1.00	42.95	15.00	56.00	3.00	67.65	0.00
30.95	1.00	44.95	2.00	57.10	7.00	67.95	1.00
34.35	1.00	46.65	0.00	58.95	1.00	71.10	1.00
34.80	0.00	47.95	1.00	59.90	2.00	72.05	1.00
35.90	1.00	48.90	18.00	60.95	26.00	73.05	17.00
36.90	23.00	49.90	259.00	61.95	85.00	74.00	106.00
37.90	60.00	50.90	770.00	63.00	249.00	75.05	83.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
76.00	104.00	89.05	144.00	101.00	19.00	113.05	1.00
77.05	1809.00	90.05	58.00	102.05	134.00	114.00	1.00
78.05	496.00	91.05	768.00	103.05	1364.00	115.05	28.00
79.05	2198.00	92.05	61.00	104.05	331.00	116.05	6.00
80.05	141.00	93.05	3.00	105.05	9999.00	117.05	11.00
81.05	4.00	94.05	2.00	106.05	1169.00	118.05	10.00
82.95	0.00	95.00	0.00	107.00	58.00	119.00	4.00
84.95	7.00	96.00	0.00	108.05	2.00	120.05	1.00
85.95	14.00	97.05	3.00	108.95	1.00	128.05	0.00
87.05	17.00	98.05	12.00	110.00	1.00	129.10	1.00
88.00	4.00	99.05	4.00	111.05	0.00	131.00	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
132.05	26.00						
134.05	1228.00						
135.05	126.00						

136.05	9.00
137.20	1.00
142.05	0.00
148.15	0.00
164.05	1.00
178.10	1.00

#115: 1,4-BENZENEDICARBOXALDEHYDE
Modified: scaled

Entry Number 115 from C:\DATABASE\hjf.l
CAS 000623-27-8
Melting Point -300
Boiling Point -300
Retention Index 70.579
Mol Formula C8H6O2
Mol Weight 134.037
Miscellaneous Information
Aldrich: terephthaldicarboxaldehyde

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	49.00	42.00	1.00	58.30	0.00	74.00	686.00
26.95	238.00	42.95	31.00	59.90	21.00	75.05	477.00
27.90	11.00	47.95	15.00	60.90	99.00	76.05	657.00
28.90	403.00	48.90	134.00	61.95	133.00	77.05	4537.00
29.95	5.00	49.90	1528.00	62.95	152.00	78.05	422.00
35.95	18.00	50.90	2967.00	64.00	16.00	79.05	23.00
36.90	173.00	52.00	378.00	65.00	3.00	80.05	1.00
37.90	220.00	52.90	126.00	65.95	22.00	83.90	10.00
38.90	225.00	53.90	5.00	66.95	16.00	84.95	38.00
39.90	8.00	55.00	10.00	71.95	10.00	86.00	47.00
40.95	1.00	57.90	0.00	72.95	153.00	87.05	26.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
88.00	7.00	100.95	6.00	120.00	2.00	143.00	1.00
89.05	42.00	102.00	3.00	127.15	0.00	150.05	0.00
90.05	7.00	103.05	81.00	128.05	0.00	153.10	3.00
91.00	1.00	104.05	218.00	128.90	0.00	154.15	1.00
91.80	0.00	105.05	5331.00	129.15	1.00	155.10	11.00
92.15	0.00	106.05	439.00	130.15	1.00	156.10	2.00
95.00	1.00	107.05	28.00	133.05	8494.00	165.10	4.00
96.80	0.00	108.05	2.00	134.05	9999.00	183.10	2.00
97.05	1.00	115.10	2.00	135.05	910.00		
98.00	3.00	117.05	2.00	136.05	73.00		
99.05	0.00	119.00	0.00	137.05	6.00		

#116: 2-HYDROXY-5-METHOXYBENZALDEHYDE

Modified: scaled

Entry Number 116 from C:\DATABASE\hjf.l
CAS 000672-13-9
Melting Point -300
Boiling Point -300
Retention Index 72.319
Mol Formula C8H8O3
Mol Weight 152.046

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	196.00	37.90	181.00	49.90	234.00	60.90	105.00
26.90	432.00	38.90	533.00	50.90	417.00	61.90	224.00
27.90	25.00	40.00	42.00	52.00	627.00	63.00	511.00
28.90	337.00	40.90	188.00	53.00	1901.00	64.05	150.00
29.95	12.00	41.90	36.00	53.90	303.00	65.00	374.00
30.95	22.00	43.00	37.00	54.90	807.00	66.00	110.00
32.95	2.00	44.90	9.00	56.00	31.00	67.05	82.00
33.95	0.00	45.95	15.00	57.05	8.00	68.05	19.00
35.05	1.00	46.95	23.00	58.00	2.00	68.90	175.00
35.90	9.00	47.90	4.00	59.00	8.00	69.95	10.00
36.90	89.00	48.90	34.00	59.90	15.00	71.05	7.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
72.00	3.00	83.05	19.00	95.00	491.00	108.05	380.00
73.00	20.00	85.05	4.00	96.00	50.00	109.05	1603.00
74.00	88.00	85.90	0.00	97.05	8.00	110.05	108.00
75.00	91.00	87.05	1.00	98.05	2.00	111.05	11.00
76.05	67.00	87.90	0.00	99.00	2.00	112.00	1.00
77.05	71.00	89.05	2.00	101.00	2.00	113.10	2.00
78.05	19.00	90.00	11.00	103.05	3.00	119.00	26.00
79.05	222.00	91.00	76.00	104.05	5.00	120.05	13.00
80.00	207.00	92.05	85.00	105.05	4.00	121.05	56.00
81.05	1342.00	93.00	147.00	106.05	522.00	122.05	59.00
82.05	121.00	94.05	38.00	107.05	273.00	123.05	452.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
124.05	67.00	145.15	2.00				
125.05	9.00	147.05	0.00				
126.10	1.00	148.05	0.00				
132.05	1.00	149.05	11.00				
133.05	2.00	150.00	165.00				
134.05	124.00	151.05	1545.00				
135.05	100.00	152.05	9999.00				
137.05	5906.00	153.05	885.00				
138.05	446.00	154.05	93.00				
139.05	50.00	155.05	6.00				
140.05	3.00	169.00	0.00				

#117: 2,3-DIHYDROXYBENZALDEHYDE
Modified: scaled

Entry Number 117 from C:\DATABASE\hjf.l
CAS 024677-78-9
Melting Point -300
Boiling Point -300
Retention Index 64.06
Mol Formula C7H6O3
Mol Weight 138.032

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	139.00	38.90	534.00	52.90	1143.00	64.90	187.00
26.90	626.00	40.05	80.00	54.00	285.00	65.90	98.00
28.90	377.00	41.90	76.00	54.95	940.00	67.00	26.00
29.95	16.00	43.00	48.00	55.90	36.00	68.90	231.00
30.95	44.00	44.90	17.00	57.05	14.00	71.00	15.00
31.90	13.00	45.95	146.00	58.00	10.00	72.00	5.00
34.00	3.00	48.00	16.00	59.95	28.00	72.95	12.00
35.10	3.00	48.90	124.00	60.90	122.00	74.00	40.00
35.90	24.00	49.90	446.00	61.95	271.00	75.00	20.00
36.90	165.00	50.95	556.00	63.05	1155.00	76.00	7.00
37.90	299.00	52.05	469.00	64.05	1220.00	76.95	75.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
78.05	17.00	90.00	17.00	101.90	1.00	115.05	2.00
79.05	178.00	91.05	220.00	103.05	2.00	118.05	1.00
80.05	191.00	92.05	2255.00	104.05	4.00	119.05	119.00
81.05	1980.00	93.05	165.00	105.05	2.00	120.05	1350.00
82.05	255.00	93.95	11.00	107.05	448.00	121.05	109.00
83.05	18.00	94.95	7.00	108.05	227.00	122.00	11.00
83.95	1.00	95.90	1.00	109.05	1373.00	122.90	1.00
85.00	3.00	97.05	2.00	110.05	375.00	123.10	3.00
85.90	1.00	98.15	1.00	111.05	29.00	133.05	7.00
87.05	2.00	98.90	1.00	112.10	6.00	134.05	6.00
89.00	1.00	99.15	1.00	113.05	1.00	136.05	308.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
137.05	7059.00	179.05	1.00				
138.05	9999.00	193.00	6.00				
139.05	812.00	194.00	6.00				
140.05	88.00						
141.05	9.00						
148.05	5.00						
150.05	1.00						
151.10	7.00						
152.10	5.00						
162.95	1.00						
169.00	1.00						

#118: 3-HYDROXYBENZALDEHYDE
Modified: scaled

Entry Number 118 from C:\DATABASE\hjf.l
CAS 000100-83-4
Melting Point -300
Boiling Point -300
Retention Index 82.819
Mol Formula C7H6O2
Mol Weight 122.037

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	62.00	39.90	338.00	52.90	397.00	67.00	67.00
26.90	131.00	40.90	25.00	53.90	33.00	68.05	26.00
28.90	236.00	41.90	50.00	54.90	213.00	72.00	5.00
29.90	5.00	43.00	42.00	56.00	6.00	73.00	49.00
31.00	45.00	44.95	4.00	60.05	23.00	74.05	187.00
34.00	0.00	45.95	71.00	60.90	190.00	75.05	115.00
34.55	1.00	47.90	10.00	61.95	324.00	76.05	94.00
35.90	23.00	48.90	70.00	62.95	793.00	77.05	60.00
36.90	232.00	49.90	359.00	64.05	393.00	78.05	7.00
37.90	502.00	50.95	295.00	65.05	2933.00	78.95	21.00
38.90	2082.00	52.05	54.00	66.05	701.00	80.00	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
84.00	2.00	95.05	43.00	117.05	1.00	145.05	0.00
85.05	7.00	96.05	2.00	119.05	24.00	147.05	7.00
85.95	6.00	99.10	1.00	121.05	8034.00	148.05	1.00
87.00	3.00	100.95	2.00	122.05	9999.00	149.15	0.00
88.05	1.00	103.00	2.00	123.05	811.00	150.05	1.00
88.95	2.00	104.05	3.00	124.05	71.00	152.20	2.00
89.95	9.00	105.05	8.00	125.05	3.00	153.05	2.00
91.05	25.00	106.05	2.00	126.10	0.00	154.30	1.00
92.05	159.00	107.05	3.00	128.05	1.00	155.05	4.00
93.05	4792.00	108.05	0.00	129.10	1.00	156.05	1.00
94.05	627.00	115.05	1.00	141.10	1.00	157.20	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
159.05	1.00						
163.05	0.00						
164.05	2.00						
168.20	1.00						
169.05	7.00						
170.10	5.00						
171.05	1.00						
187.05	3.00						
195.05	1.00						
197.05	3.00						
220.20	1.00						

#119: 3-ETHOXY-4-HYDROXYBENZALDEHYDE
Modified: scaled

Entry Number 119 from C:\DATABASE\hjf.l
CAS 000100-83-4
Melting Point -300
Boiling Point -300
Retention Index 83.65
Mol Formula C9H10O3
Mol Weight 166.062

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	109.00	38.90	339.00	50.90	464.00	62.95	327.00
26.90	753.00	39.90	20.00	51.95	377.00	64.05	195.00
27.90	54.00	40.95	29.00	52.90	642.00	65.05	199.00
28.90	852.00	41.90	23.00	54.05	103.00	66.00	45.00
29.95	22.00	42.90	83.00	54.90	230.00	67.00	38.00
30.90	16.00	44.90	47.00	56.00	11.00	68.05	9.00
32.80	0.00	45.95	2.00	57.05	24.00	68.90	10.00
32.90	0.00	46.90	3.00	58.00	3.00	70.05	3.00
36.00	2.00	47.90	2.00	59.90	3.00	71.05	11.00
36.90	36.00	48.90	28.00	60.90	30.00	72.00	1.00
37.90	110.00	49.90	228.00	61.95	100.00	72.95	4.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
74.00	22.00	85.05	5.00	96.05	8.00	107.05	68.00
75.00	47.00	85.95	0.00	97.05	2.00	108.05	125.00
76.00	9.00	87.00	1.00	98.10	0.00	109.05	1424.00
77.05	59.00	88.05	0.00	99.10	1.00	110.05	364.00
78.05	14.00	89.00	2.00	101.05	1.00	111.05	30.00
79.05	212.00	90.05	7.00	101.90	0.00	112.10	3.00
80.05	124.00	91.05	150.00	102.10	1.00	113.10	2.00
81.05	947.00	92.05	112.00	103.05	2.00	115.10	0.00
82.05	217.00	93.05	7.00	104.05	1.00	117.05	1.00
83.05	14.00	94.05	11.00	105.05	4.00	118.10	1.00
83.95	1.00	95.05	41.00	106.05	1.00	119.05	40.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
120.05	24.00	135.05	9.00	150.05	5.00	169.00	5.00
123.05	28.00	137.05	9999.00	151.05	4.00	170.05	1.00
124.05	4.00	138.05	3532.00	152.05	1.00	180.10	0.00
125.05	1.00	139.05	311.00	155.15	1.00	182.15	0.00
126.05	0.00	140.05	30.00	161.10	1.00	183.15	1.00
127.10	0.00	141.05	3.00	162.05	0.00	194.05	0.00
128.15	0.00	143.10	1.00	163.05	5.00	197.25	0.00
130.15	0.00	145.05	1.00	164.10	4.00	201.05	0.00
131.90	0.00	147.05	3.00	166.05	5217.00	207.05	0.00
132.05	0.00	148.05	1.00	167.05	582.00	225.30	0.00

133.05	0.00	149.05	37.00	168.05	62.00	229.05	0.00

#120: 1,4-BENZOQUINONE
Modified: scaled

Entry Number 120 from C:\DATABASE\hjf.l
CAS 000106-51-4
Melting Point -300
Boiling Point -300
Retention Index 44.09
Mol Formula C6H4O2
Mol Weight 108.021

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	3247.00	38.90	83.00	49.90	659.00	61.95	182.00
26.90	185.00	39.90	17.00	50.95	465.00	62.95	138.00
27.90	101.00	40.90	178.00	51.90	1842.00	64.00	32.00
28.90	86.00	41.90	23.00	52.90	1798.00	65.00	9.00
30.90	75.00	43.05	13.00	53.90	7437.00	66.00	8.00
33.30	1.00	44.90	1.00	54.90	348.00	66.95	2.00
33.55	0.00	45.90	1.00	56.00	26.00	68.00	4.00
34.40	0.00	46.90	1.00	57.05	16.00	71.05	6.00
35.85	89.00	47.05	0.00	58.05	1.00	71.95	7.00
36.85	280.00	47.85	53.00	59.90	87.00	72.95	20.00
37.90	195.00	48.90	238.00	60.85	236.00	73.95	21.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
74.95	4.00	85.05	7.00	98.15	0.00	111.05	36.00
75.90	2.00	85.90	1.00	99.05	3.00	112.10	4.00
76.15	0.00	86.05	1.00	100.95	0.00	113.10	2.00
76.95	16.00	86.90	0.00	102.10	1.00	117.90	0.00
78.05	5.00	90.00	1.00	103.90	0.00	120.05	1.00
79.00	85.00	91.00	1.00	104.15	0.00	121.05	0.00
80.05	3479.00	92.00	3.00	105.00	1.00	121.90	0.00
81.00	303.00	93.00	2.00	106.10	5.00	131.95	1.00
81.90	3472.00	94.05	5.00	108.05	9999.00	134.05	15.00
83.00	156.00	95.05	3.00	109.05	698.00	135.05	3.00
83.95	17.00	96.00	1.00	110.05	532.00	136.05	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
141.20	0.00						
146.80	0.00						
160.10	2.00						
161.05	0.00						
163.95	0.00						
171.00	1.00						
188.05	4.00						

#121: 1-(2,5-DIHYDROXYPHENYL)-ETHANONE
Modified: scaled

Entry Number 121 from C:\DATABASE\hjf.l
CAS 000490-78-8
Melting Point -300
Boiling Point -300
Retention Index 87.109
Mol Formula C8H8O3
Mol Weight 152.046
Miscellaneous Information
Aldrich: 2',5'-dihydroxyacetophenone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	147.00	38.90	379.00	52.00	466.00	66.05	72.00
26.90	425.00	39.90	52.00	52.90	1095.00	67.05	108.00
28.90	137.00	41.00	118.00	54.00	310.00	68.90	558.00
29.95	4.00	41.95	103.00	54.90	382.00	70.00	20.00
30.90	12.00	42.90	1453.00	56.05	15.00	73.00	10.00
32.80	1.00	44.90	16.00	59.90	7.00	74.00	31.00
33.95	3.00	45.90	8.00	60.90	60.00	75.05	20.00
34.90	8.00	47.00	13.00	62.00	111.00	76.05	90.00
35.90	5.00	48.90	49.00	63.00	216.00	77.05	268.00
36.90	57.00	49.90	207.00	64.05	49.00	78.05	246.00
37.90	110.00	50.90	436.00	65.05	83.00	79.05	102.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
80.05	140.00	93.05	16.00	108.05	194.00	122.05	2.00
81.05	1596.00	94.05	16.00	109.05	2396.00	123.05	51.00
82.05	211.00	95.05	66.00	110.05	284.00	124.05	7.00
83.05	14.00	96.05	6.00	111.05	24.00	125.10	1.00
86.05	6.00	97.05	6.00	112.05	3.00	128.10	0.00
87.00	4.00	98.05	2.00	115.05	0.00	133.05	107.00
88.05	2.00	101.05	1.00	116.05	1.00	134.05	384.00
89.05	4.00	103.05	1.00	117.05	1.00	135.05	40.00
90.05	6.00	105.05	174.00	119.05	1.00	137.05	9999.00
91.05	17.00	106.05	108.00	120.05	2.00	138.05	778.00
92.05	23.00	107.05	23.00	121.05	15.00	139.05	93.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
140.05	5.00	155.05	5.00	193.05	1.00	226.10	1.00
142.15	1.00	156.20	0.00	194.00	1.00	228.05	0.00
145.05	0.00	159.05	0.00	195.10	1.00	238.30	0.00
147.05	0.00	161.10	0.00	196.20	0.00	239.30	0.00
148.10	1.00	163.05	1.00	206.20	0.00		
149.10	19.00	165.05	0.00	208.10	0.00		
150.05	5.00	166.15	0.00	211.05	2.00		
151.10	125.00	173.05	0.00	213.05	0.00		
152.05	7638.00	175.05	1.00	220.15	1.00		
153.05	717.00	176.05	0.00	224.30	0.00		

154.05	77.00	179.05	1.00	225.20	0.00

#122: 3-FUROIC ACID
Modified: scaled

Entry Number 122 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 57.149
Mol Formula C5H4O3
Mol Weight 112.016

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	101.00	35.85	111.00	47.40	161.00	59.05	0.00
26.95	161.00	36.90	738.00	48.90	49.00	59.65	1.00
27.90	226.00	37.90	1427.00	49.85	54.00	60.00	8.00
28.90	706.00	38.90	3204.00	50.90	13.00	60.85	2.00
29.95	20.00	39.90	190.00	52.00	28.00	61.05	1.00
30.95	5.00	40.90	82.00	52.85	179.00	61.30	1.00
31.90	2.00	41.90	129.00	54.05	29.00	63.00	3.00
33.00	11.00	43.00	7.00	54.90	591.00	64.00	11.00
33.45	5.00	43.90	175.00	55.95	166.00	64.95	46.00
34.35	1.00	44.90	548.00	56.95	13.00	65.90	359.00
34.90	1.00	45.95	10.00	57.95	40.00	66.90	824.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
67.90	130.00	79.05	6.00	93.00	11.00	113.00	550.00
68.90	41.00	80.65	1.00	94.95	8786.00	113.95	76.00
69.90	6.00	80.95	1.00	96.00	506.00	114.95	6.00
71.00	2.00	82.00	9.00	96.95	52.00	118.95	1.00
71.90	1.00	82.95	72.00	98.05	2.00	122.00	5.00
73.00	4.00	83.90	276.00	101.05	1.00	130.95	3.00
75.85	1.00	85.00	20.00	104.40	1.00	149.95	7.00
76.15	1.00	85.90	12.00	105.05	14.00	164.05	1.00
77.00	12.00	87.90	1.00	106.05	1.00	169.00	1.00
77.90	6.00	90.95	9.00	110.15	1.00	218.95	1.00
78.85	2.00	92.00	2.00	112.05	9999.00		

#123: 2-FUROIC ACID
Modified: scaled

Entry Number 123 from C:\DATABASE\hjf.l
CAS 000088-14-2
Melting Point -300
Boiling Point -300
Retention Index 64.829

Mol Formula C5H4O3
Mol Weight 112.016

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.90	144.00	38.90	3734.00	48.95	44.00	59.95	26.00
26.95	198.00	39.90	358.00	49.95	44.00	60.95	3.00
27.90	361.00	40.95	186.00	50.95	107.00	64.00	18.00
28.90	575.00	41.90	339.00	52.00	28.00	65.00	45.00
29.95	16.00	42.90	2.00	52.90	191.00	65.95	179.00
33.30	66.00	43.90	282.00	53.95	47.00	66.90	718.00
34.75	5.00	44.90	654.00	54.90	597.00	67.95	163.00
34.95	7.00	45.80	6.00	56.00	184.00	68.90	19.00
35.90	107.00	46.05	9.00	56.90	20.00	69.95	12.00
36.90	721.00	47.40	44.00	58.00	13.00	70.90	5.00
37.90	1375.00	47.65	12.00	58.95	2.00	72.95	17.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
75.85	5.00	83.00	60.00	95.05	7434.00	114.00	74.00
76.05	2.00	84.00	528.00	96.05	442.00	115.00	4.00
76.95	28.00	84.95	38.00	96.95	51.00	119.00	3.00
78.05	17.00	85.90	11.00	98.05	2.00	122.05	15.00
78.95	9.00	86.90	2.00	99.90	1.00	130.90	1.00
79.10	8.00	87.90	2.00	100.95	6.00	132.00	8.00
80.15	2.00	89.30	2.00	104.15	2.00	150.00	18.00
80.80	2.00	89.90	2.00	105.05	33.00	168.95	1.00
80.90	2.00	91.00	17.00	106.00	5.00	218.95	5.00
81.05	6.00	91.95	3.00	112.00	9999.00		
81.95	6.00	93.00	27.00	113.05	581.00		

#124: HEXANAL
Modified: scaled

Entry Number 124 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 28.739
Mol Formula C6H12O
Mol Weight 100.088

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.10	2.00	36.95	67.00	48.05	4.00	59.00	54.00
26.00	389.00	38.00	177.00	49.00	8.00	60.00	5.00
27.00	4690.00	39.00	2315.00	50.00	76.00	61.00	9.00
28.00	1164.00	40.00	475.00	51.00	108.00	61.95	13.00
29.00	5584.00	41.00	7503.00	51.95	33.00	62.95	17.00
30.00	210.00	42.00	1264.00	53.00	267.00	63.95	5.00
31.00	223.00	43.00	5543.00	54.00	217.00	65.05	36.00

32.95	5.00	44.00	9999.00	55.05	1345.00	66.00	13.00
34.05	5.00	45.00	1982.00	56.10	6979.00	67.05	775.00
35.05	1.00	46.00	60.00	57.00	4481.00	68.05	54.00
35.95	3.00	47.00	5.00	58.00	786.00	69.00	83.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
70.05	49.00	79.05	23.00	88.80	0.00	94.90	0.00
71.10	545.00	80.10	4.00	89.10	1.00	95.25	1.00
72.10	1430.00	81.10	93.00	89.75	0.00	96.05	1.00
73.05	66.00	82.10	922.00	90.10	0.00	97.00	2.00
74.00	6.00	83.10	107.00	90.40	0.00	97.50	0.00
75.00	1.00	84.00	5.00	91.05	1.00	98.15	3.00
75.55	0.00	85.05	18.00	91.40	0.00	99.15	15.00
75.75	0.00	85.95	0.00	92.00	0.00	100.10	19.00
76.10	0.00	87.40	0.00	92.20	1.00	101.10	12.00
77.00	8.00	87.70	1.00	93.00	1.00	102.00	0.00
78.05	1.00	88.15	0.00	94.05	1.00	102.25	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
102.95	0.00	108.50	0.00	116.50	0.00	125.10	0.00
103.20	0.00	110.00	0.00	118.05	0.00	125.95	0.00
103.90	0.00	110.65	0.00	119.05	1.00	126.75	0.00
104.10	0.00	111.40	0.00	121.25	0.00	127.20	0.00
104.50	0.00	111.65	0.00	122.25	0.00	127.75	0.00
104.75	0.00	112.15	0.00	122.50	0.00	128.20	1.00
105.20	0.00	112.40	0.00	122.90	0.00	129.05	1.00
106.15	1.00	113.65	0.00	124.00	0.00	129.65	0.00
106.50	0.00	114.20	1.00	124.15	0.00	130.15	0.00
106.85	0.00	115.10	1.00	124.40	0.00	131.00	0.00
107.60	1.00	115.75	0.00	124.75	0.00	132.80	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
134.15	0.00	145.05	0.00	154.85	0.00	167.60	0.00
134.85	0.00	146.15	0.00	156.25	0.00	168.30	0.00
135.15	0.00	146.95	1.00	158.20	0.00	170.55	0.00
135.55	0.00	148.90	0.00	159.15	0.00	171.90	0.00
136.70	0.00	149.15	0.00	159.40	0.00	172.30	0.00
137.30	0.00	150.05	0.00	162.15	0.00	173.65	0.00
138.30	0.00	150.80	0.00	163.05	0.00	177.05	0.00
140.80	0.00	152.90	0.00	164.05	1.00	179.15	0.00
141.05	0.00	153.30	0.00	165.90	0.00	179.40	0.00
141.65	0.00	153.90	0.00	166.55	0.00	180.65	0.00
143.15	0.00	154.30	0.00	166.80	0.00	184.15	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
184.40	0.00	200.05	0.00	209.70	0.00	223.30	0.00
185.30	0.00	200.70	0.00	210.05	0.00	223.55	0.00
186.30	0.00	200.95	0.00	211.95	0.00	225.80	0.00
188.05	0.00	202.05	0.00	212.30	0.00	227.95	0.00
188.35	0.00	202.55	0.00	214.00	0.00	228.80	0.00
189.05	0.00	202.95	0.00	216.00	0.00	230.70	0.00
189.45	0.00	203.55	0.00	218.05	0.00	231.00	0.00

191.80	0.00	205.30	0.00	219.80	0.00	231.30	0.00
195.80	0.00	205.55	0.00	221.25	0.00	233.45	0.00
198.45	0.00	207.45	0.00	222.55	0.00	234.95	0.00
199.80	0.00	208.55	0.00	223.05	0.00	235.80	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
240.30	0.00						
243.20	0.00						
246.10	0.00						

#125: HEPTANAL
Modified: scaled

Entry Number 125 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 37.609
Mol Formula C7H14O
Mol Weight 114.103

N	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	357.00	37.00	44.00	47.85	2.00	58.95	45.00
27.00	4964.00	38.00	140.00	49.00	4.00	60.05	1.00
28.00	1178.00	39.00	2646.00	49.95	82.00	61.00	4.00
29.00	6980.00	40.00	419.00	51.00	137.00	62.05	11.00
30.00	220.00	41.00	7796.00	52.00	45.00	63.00	17.00
31.00	272.00	42.00	5772.00	53.00	389.00	64.00	3.00
33.00	4.00	43.00	8669.00	54.00	633.00	64.95	73.00
33.95	4.00	44.00	9999.00	55.05	5133.00	66.00	70.00
34.75	3.00	45.00	2179.00	56.10	600.00	67.10	672.00
35.75	1.00	46.00	65.00	57.00	4336.00	68.05	1222.00
36.00	2.00	47.05	5.00	58.00	525.00	69.05	379.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
70.10	6616.00	82.15	108.00	90.25	0.00	100.85	1.00
71.10	1961.00	83.15	54.00	91.00	4.00	101.00	0.00
72.10	753.00	84.10	18.00	92.00	0.00	102.95	1.00
73.05	41.00	85.10	237.00	92.20	2.00	103.70	1.00
74.00	32.00	86.15	992.00	93.15	8.00	104.00	0.00
75.05	3.00	87.15	55.00	94.20	2.00	104.65	0.00
76.15	1.00	88.10	3.00	95.15	91.00	105.15	1.00
76.95	19.00	88.95	1.00	96.15	657.00	105.50	0.00
78.10	4.00	89.15	0.00	97.15	109.00	107.75	0.00
79.10	71.00	89.50	0.00	98.15	6.00	108.05	1.00
81.15	1576.00	89.75	0.00	99.15	20.00	108.40	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
108.75	0.00	119.75	0.00	126.25	0.00	137.40	0.00
109.00	1.00	119.90	0.00	126.95	1.00	138.15	0.00

110.10	1.00	120.10	0.00	127.15	0.00	138.55	0.00
110.90	1.00	121.15	0.00	128.15	1.00	139.40	0.00
112.10	1.00	122.50	0.00	128.25	0.00	140.10	0.00
113.15	15.00	123.65	0.00	128.65	0.00	140.55	0.00
114.15	37.00	123.90	0.00	129.20	0.00	140.80	0.00
115.15	16.00	124.15	0.00	132.80	0.00	142.90	0.00
116.25	1.00	125.25	0.00	134.05	0.00	143.15	0.00
118.15	0.00	125.50	0.00	135.55	0.00	145.05	0.00
118.40	0.00	126.00	1.00	136.15	0.00	145.40	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
146.30	0.00	161.60	0.00	173.90	0.00	192.80	0.00
147.05	0.00	163.80	0.00	174.65	0.00	195.05	0.00
148.15	0.00	164.15	0.00	175.40	0.00	197.70	0.00
148.40	0.00	164.80	0.00	176.35	0.00	198.55	0.00
148.90	0.00	165.05	0.00	176.65	0.00	203.05	0.00
150.10	1.00	166.90	0.00	179.30	0.00	205.00	0.00
154.05	0.00	167.15	0.00	179.65	0.00	206.40	0.00
154.65	0.00	167.55	0.00	181.05	0.00	207.15	0.00
158.90	0.00	169.05	1.00	181.30	0.00	208.80	0.00
160.80	0.00	171.05	1.00	190.70	0.00	215.20	0.00
161.30	0.00	173.40	0.00	191.80	0.00	220.20	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
220.45	0.00						
225.70	0.00						
225.95	0.00						
228.30	0.00						
232.95	0.00						
237.80	0.00						

#126: OCTANAL
Modified: scaled

Entry Number 126 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 45.969
Mol Formula C8H16O
Mol Weight 128.12

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	265.00	36.00	1.00	45.00	1992.00	55.00	4519.00
27.00	4563.00	36.10	1.00	46.00	59.00	56.10	6407.00
28.00	956.00	36.25	1.00	47.00	7.00	57.00	5862.00
29.00	7110.00	37.00	28.00	47.85	1.00	58.00	517.00
30.00	209.00	38.05	105.00	48.00	0.00	59.00	62.00
31.00	252.00	39.00	2596.00	49.00	0.00	60.00	3.00

33.05	4.00	40.00	465.00	50.00	52.00	61.05	3.00
34.00	1.00	41.00	8404.00	51.00	124.00	62.00	8.00
34.25	1.00	42.00	4244.00	52.00	49.00	62.95	16.00
34.75	0.00	43.05	9999.00	53.00	450.00	63.90	5.00
35.75	1.00	44.00	7945.00	54.00	701.00	65.00	81.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
66.05	405.00	76.05	0.00	87.15	14.00	98.15	11.00
67.10	1688.00	77.05	31.00	88.00	1.00	99.15	158.00
68.05	1954.00	78.05	6.00	89.10	0.00	100.15	622.00
69.05	2768.00	79.10	153.00	89.65	0.00	101.15	41.00
70.05	271.00	80.15	72.00	90.25	0.00	102.05	2.00
71.05	798.00	81.10	1584.00	91.15	8.00	103.15	0.00
72.05	699.00	82.15	1602.00	92.05	1.00	103.85	0.00
73.05	47.00	83.10	204.00	93.15	17.00	104.15	0.00
74.05	18.00	84.15	3331.00	95.15	508.00	104.45	0.00
75.10	2.00	85.15	1160.00	96.10	44.00	104.75	0.00
75.35	0.00	86.10	164.00	97.10	29.00	104.95	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
106.15	1.00	116.40	0.00	125.00	0.00	137.30	0.00
107.10	2.00	117.40	0.00	126.20	1.00	139.30	0.00
107.75	0.00	117.90	0.00	127.15	10.00	139.55	0.00
108.00	0.00	120.20	1.00	128.15	13.00	139.80	0.00
109.15	40.00	120.65	0.00	129.15	12.00	140.30	0.00
110.15	309.00	120.95	0.00	130.25	2.00	140.55	0.00
111.15	50.00	121.30	1.00	133.40	0.00	140.85	0.00
112.20	2.00	122.50	0.00	134.05	0.00	141.15	0.00
113.15	11.00	123.00	0.00	135.20	1.00	142.15	0.00
114.15	0.00	123.40	0.00	136.30	0.00	142.65	0.00
115.00	1.00	123.90	0.00	136.80	0.00	143.05	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
144.80	0.00	156.15	0.00	170.35	0.00	190.20	0.00
145.15	0.00	156.55	0.00	171.55	0.00	190.45	0.00
145.55	0.00	157.55	0.00	172.15	0.00	190.80	0.00
145.80	0.00	158.25	0.00	175.05	0.00	192.45	0.00
146.15	0.00	161.80	0.00	176.15	0.00	196.30	0.00
147.05	0.00	163.15	0.00	178.80	0.00	198.70	0.00
148.55	0.00	164.40	0.00	179.05	0.00	198.95	0.00
149.80	0.00	164.90	0.00	180.40	0.00	201.05	0.00
149.90	0.00	166.65	0.00	181.05	1.00	204.95	0.00
151.05	0.00	167.15	0.00	181.30	0.00	206.45	0.00
155.05	0.00	169.05	2.00	182.35	0.00	207.05	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
208.95	0.00	247.95	0.00				
209.80	0.00						
211.75	0.00						
214.00	0.00						
214.80	0.00						
220.15	0.00						

222.20	0.00
225.30	0.00
225.55	0.00
228.20	0.00
238.00	0.00

#127: NONANAL
Modified: scaled

Entry Number 127 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 53.789
Mol Formula C9H18O
Mol Weight 142.134

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	226.00	39.00	2440.00	50.00	43.00	61.05	2.00
27.00	4275.00	40.00	444.00	51.00	110.00	61.30	0.00
28.00	861.00	41.00	9454.00	52.00	47.00	61.95	5.00
29.00	7244.00	42.00	2923.00	53.00	493.00	62.95	15.00
29.95	190.00	43.00	7814.00	54.05	1348.00	64.00	4.00
31.00	235.00	44.00	6708.00	55.05	4802.00	65.05	86.00
33.75	2.00	45.00	1883.00	56.10	6507.00	66.00	316.00
33.85	1.00	46.00	55.00	57.00	9999.00	67.05	1909.00
36.00	1.00	47.00	5.00	58.00	684.00	68.05	2559.00
37.00	20.00	48.05	3.00	59.05	66.00	69.05	2766.00
38.05	80.00	49.00	1.00	60.00	2.00	70.05	3620.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
71.10	1333.00	81.15	1815.00	94.15	57.00	103.90	1.00
72.05	633.00	82.15	2329.00	95.15	1376.00	105.15	1.00
73.10	57.00	83.10	775.00	96.15	1348.00	106.05	0.00
74.00	3.00	84.15	83.00	97.10	136.00	107.15	3.00
75.10	0.00	85.15	232.00	98.15	2060.00	109.15	125.00
75.60	0.00	86.10	179.00	99.15	362.00	110.15	13.00
76.05	1.00	87.15	12.00	100.10	40.00	111.20	12.00
77.05	38.00	88.25	1.00	101.10	3.00	112.20	4.00
78.15	9.00	88.85	0.00	102.20	0.00	113.15	41.00
79.15	176.00	91.05	13.00	103.10	1.00	114.10	389.00
80.15	81.00	93.10	38.00	103.65	0.00	115.15	26.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
116.20	2.00	126.40	1.00	136.15	0.00	145.15	0.00
117.40	0.00	127.20	6.00	136.90	0.00	145.90	0.00
117.75	0.00	128.10	1.00	137.30	0.00	147.00	0.00
119.00	2.00	128.75	0.00	138.05	1.00	149.05	0.00
120.40	0.00	129.00	0.00	139.05	0.00	151.10	0.00

121.10	1.00	129.25	0.00	139.40	0.00	153.90	0.00
121.75	0.00	130.15	0.00	140.30	1.00	154.65	0.00
123.20	12.00	132.20	0.00	141.20	9.00	155.30	0.00
124.15	137.00	132.90	0.00	142.20	6.00	157.15	0.00
125.20	15.00	133.20	0.00	143.15	10.00	158.15	0.00
126.15	1.00	133.55	0.00	144.25	1.00	164.80	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
165.05	0.00	188.80	0.00	224.95	0.00		
168.05	0.00	192.80	0.00	226.70	0.00		
168.95	1.00	195.20	0.00	232.05	0.00		
170.05	0.00	198.80	0.00	232.30	0.00		
176.10	0.00	202.95	0.00	236.20	0.00		
176.40	0.00	205.95	0.00	246.35	0.00		
178.30	0.00	206.45	0.00				
178.90	0.00	207.30	0.00				
184.55	0.00	215.95	0.00				
184.90	0.00	218.05	0.00				
187.50	0.00	220.05	0.00				

#128: DECANAL
Modified: scaled

Entry Number 128 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 61.1
Mol Formula C10H20O
Mol Weight 156.151

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	193.00	37.00	14.00	47.90	2.00	60.00	2.00
27.00	4127.00	38.05	16.00	50.00	32.00	61.25	1.00
28.00	778.00	39.00	2341.00	51.00	97.00	62.00	4.00
29.00	7276.00	40.05	436.00	52.05	44.00	63.00	12.00
30.00	192.00	41.00	9426.00	53.00	544.00	64.00	5.00
31.00	231.00	42.00	3380.00	54.00	1422.00	65.00	102.00
32.95	2.00	43.00	9999.00	55.00	6085.00	66.00	545.00
34.00	1.00	44.00	6114.00	56.05	4106.00	67.05	2978.00
34.75	0.00	45.00	1843.00	57.05	8778.00	68.10	3478.00
35.10	0.00	46.00	52.00	58.00	602.00	69.05	2596.00
35.60	0.00	47.00	10.00	59.05	73.00	70.10	4190.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
71.10	3636.00	82.15	3449.00	91.15	19.00	101.90	1.00
72.10	790.00	83.15	2576.00	92.15	3.00	102.20	1.00
73.05	64.00	84.10	1416.00	93.15	53.00	102.95	1.00
74.05	5.00	85.10	368.00	94.20	68.00	103.20	0.00

74.95	1.00	86.10	133.00	95.15	1498.00	103.75	0.00
76.05	1.00	87.15	13.00	96.15	1363.00	104.00	0.00
77.05	46.00	88.15	1.00	97.10	431.00	104.35	0.00
78.15	10.00	88.90	0.00	98.10	45.00	105.15	0.00
79.15	218.00	89.20	1.00	99.10	185.00	105.80	0.00
80.15	125.00	89.65	0.00	100.10	89.00	107.15	7.00
81.15	2289.00	89.95	1.00	101.10	6.00	108.15	8.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
109.15	592.00	119.90	0.00	130.20	2.00	140.35	1.00
110.15	900.00	121.15	1.00	132.00	0.00	141.20	4.00
111.20	88.00	122.15	1.00	133.05	0.00	142.35	1.00
112.10	1339.00	123.15	43.00	133.30	0.00	144.30	0.00
113.15	165.00	124.20	5.00	134.05	0.00	144.80	0.00
114.10	18.00	125.20	4.00	135.20	0.00	145.05	0.00
115.20	2.00	126.00	1.00	136.30	1.00	145.30	0.00
116.00	1.00	126.20	0.00	137.20	6.00	146.15	0.00
116.40	0.00	127.15	19.00	138.20	81.00	146.90	1.00
117.10	1.00	128.10	257.00	139.20	9.00	148.10	0.00
117.95	0.00	129.20	20.00	140.05	0.00	150.65	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
151.05	0.00	159.05	0.00	170.15	0.00	183.30	0.00
151.30	0.00	159.30	1.00	170.65	0.00	187.20	0.00
151.65	0.00	159.90	0.00	173.30	0.00	191.05	0.00
152.15	0.00	161.15	0.00	173.65	0.00	194.20	0.00
152.90	0.00	162.15	0.00	175.55	0.00	197.30	0.00
153.30	0.00	163.80	0.00	176.40	0.00	200.30	0.00
154.30	0.00	164.10	0.00	177.15	0.00	204.45	0.00
155.25	8.00	164.40	0.00	177.40	0.00	205.55	0.00
156.20	5.00	168.15	0.00	179.10	0.00	207.05	0.00
157.30	12.00	168.35	0.00	180.15	0.00	208.20	0.00
158.25	1.00	169.90	0.00	180.95	0.00	208.65	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
209.80	0.00	234.45	0.00				
210.80	0.00	240.30	0.00				
211.55	0.00	242.50	0.00				
216.55	0.00						
220.00	0.00						
221.55	0.00						
225.95	0.00						
226.30	0.00						
227.70	0.00						
231.05	0.00						
232.30	0.00						

#129: HEXANOIC ACID
Modified: scaled

Entry Number 129 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 52.409
Mol Formula C6H12O2
Mol Weight 116.082

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	285.00	35.25	0.00	46.00	56.00	57.10	1062.00
27.00	2738.00	36.00	9.00	47.00	41.00	58.05	58.00
28.00	860.00	37.00	40.00	48.00	16.00	60.00	9999.00
29.00	2283.00	38.00	113.00	48.95	3.00	61.00	935.00
30.00	168.00	39.00	1406.00	50.00	40.00	62.00	69.00
31.00	259.00	40.00	243.00	51.00	61.00	62.95	14.00
32.00	9.00	41.00	3508.00	52.00	17.00	63.95	7.00
33.00	8.00	42.00	1796.00	53.00	154.00	65.00	14.00
33.95	8.00	43.00	2622.00	54.05	66.00	65.95	11.00
34.80	1.00	44.00	495.00	55.00	1419.00	67.05	34.00
35.00	2.00	45.00	1682.00	56.10	1026.00	68.00	37.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
69.00	276.00	81.10	10.00	92.25	1.00	101.05	6.00
70.10	294.00	82.05	3.00	92.40	1.00	102.05	2.00
71.05	64.00	83.10	61.00	93.15	1.00	102.40	0.00
73.00	3562.00	84.15	6.00	93.90	1.00	103.15	1.00
74.05	456.00	85.00	15.00	94.15	0.00	104.40	0.00
75.05	38.00	87.10	882.00	95.15	2.00	105.10	2.00
76.05	4.00	88.10	56.00	96.10	4.00	105.95	1.00
77.05	5.00	89.05	8.00	97.10	27.00	106.65	0.00
78.05	2.00	90.05	2.00	98.15	28.00	107.15	0.00
79.10	8.00	90.40	1.00	99.10	53.00	108.15	1.00
80.15	41.00	91.05	3.00	100.05	3.00	108.45	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
108.90	1.00	117.10	14.00	126.90	0.00	140.25	0.00
109.00	1.00	119.00	1.00	128.15	1.00	141.15	0.00
110.15	1.00	120.05	0.00	128.65	0.00	142.15	0.00
111.15	1.00	121.00	0.00	129.20	1.00	144.15	0.00
111.25	0.00	121.20	1.00	130.25	0.00	145.05	0.00
111.45	0.00	122.05	1.00	131.00	4.00	145.95	0.00
112.10	0.00	123.20	1.00	132.65	0.00	147.30	1.00
113.35	1.00	123.90	0.00	132.90	0.00	148.40	0.00
114.00	5.00	124.20	0.00	135.05	0.00	149.15	1.00
115.05	5.00	125.00	0.00	136.05	0.00	149.80	0.00
116.10	2.00	125.25	0.00	138.15	0.00	150.05	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
151.05	0.00	163.75	0.00	181.05	0.00	200.70	0.00
151.85	0.00	164.30	0.00	182.55	0.00	201.80	0.00
152.90	0.00	164.80	0.00	182.90	0.00	208.00	0.00

153.15	0.00	165.80	0.00	184.15	0.00	214.55	1.00
154.80	0.00	166.05	0.00	185.30	0.00	216.30	0.00
154.90	0.00	166.55	0.00	186.20	1.00	219.05	0.00
155.05	0.00	167.05	0.00	186.45	0.00	222.20	0.00
157.15	0.00	167.65	0.00	187.20	0.00	231.05	0.00
161.90	0.00	169.05	0.00	187.95	1.00	235.05	0.00
162.30	0.00	170.10	1.00	197.55	0.00	235.80	0.00
163.35	1.00	174.55	0.00	200.45	0.00	237.55	0.00

#130: HEPTANOIC ACID
Modified: scaled

Entry Number 130 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 59.159
Mol Formula C7H14O2
Mol Weight 130.098

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	206.00	36.95	20.00	48.00	10.00	59.10	351.00
27.00	2561.00	38.00	70.00	48.95	6.00	60.00	9999.00
28.00	810.00	39.00	1345.00	50.00	34.00	61.00	1156.00
29.00	2589.00	40.00	223.00	51.00	61.00	62.00	75.00
30.00	136.00	41.00	3651.00	52.05	25.00	63.05	13.00
31.00	261.00	42.00	1383.00	53.00	194.00	64.00	1.00
32.95	7.00	43.00	4377.00	54.05	93.00	65.00	21.00
33.90	6.00	44.00	252.00	55.00	2252.00	66.00	6.00
34.60	1.00	45.00	1318.00	56.10	497.00	67.05	99.00
35.10	1.00	46.00	38.00	57.05	312.00	68.10	254.00
35.95	4.00	47.00	38.00	58.05	41.00	69.05	416.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
70.10	1328.00	82.15	9.00	93.05	1.00	104.15	0.00
71.10	1206.00	83.10	279.00	94.10	25.00	105.00	2.00
73.00	4039.00	84.15	303.00	95.15	5.00	107.00	1.00
74.00	416.00	85.15	44.00	96.15	4.00	107.15	0.00
75.05	33.00	87.15	1592.00	97.15	26.00	107.95	1.00
76.00	2.00	88.10	103.00	98.15	5.00	108.75	0.00
77.05	12.00	89.10	17.00	99.10	7.00	109.05	2.00
78.05	2.00	90.00	1.00	100.05	3.00	110.15	5.00
79.15	20.00	91.05	4.00	101.15	393.00	111.15	12.00
80.10	3.00	92.00	0.00	102.15	37.00	112.15	8.00
81.10	16.00	92.25	0.00	103.15	3.00	113.15	40.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
114.15	4.00	122.90	0.00	129.20	3.00	137.30	0.00
115.15	20.00	123.25	1.00	130.20	11.00	137.55	0.00

116.20	2.00	123.60	1.00	131.05	11.00	138.15	0.00
117.10	1.00	123.90	0.00	132.00	1.00	138.65	0.00
117.50	0.00	124.20	1.00	133.00	0.00	138.90	0.00
117.95	1.00	124.75	0.00	133.80	0.00	139.30	0.00
120.30	1.00	125.25	0.00	134.55	0.00	139.55	0.00
120.90	0.00	125.95	1.00	135.05	1.00	140.30	0.00
121.00	1.00	126.15	1.00	136.20	2.00	141.20	1.00
121.50	1.00	127.05	1.00	136.65	0.00	141.80	0.00
122.05	2.00	128.10	0.00	137.00	1.00	143.30	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
143.65	0.00	152.90	0.00	165.15	0.00	177.20	0.00
145.00	1.00	153.30	0.00	167.65	0.00	179.05	0.00
146.30	0.00	155.65	0.00	169.05	1.00	179.55	0.00
146.90	1.00	156.15	1.00	171.05	0.00	181.15	1.00
148.15	1.00	157.15	0.00	171.40	0.00	183.65	0.00
148.55	0.00	159.15	0.00	171.90	0.00	184.15	0.00
149.15	0.00	160.15	1.00	172.80	0.00	184.40	0.00
149.40	0.00	161.30	0.00	173.15	0.00	186.00	0.00
150.00	0.00	162.40	0.00	174.40	0.00	186.95	0.00
151.15	2.00	163.15	0.00	175.90	0.00	189.95	0.00
152.15	0.00	163.90	0.00	176.15	0.00	191.25	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
197.05	0.00	214.20	0.00	240.30	0.00		
200.95	0.00	215.30	0.00	249.10	0.00		
202.55	0.00	215.55	0.00				
204.95	0.00	219.05	0.00				
205.95	0.00	220.05	1.00				
206.95	0.00	220.20	1.00				
207.20	0.00	225.45	0.00				
208.05	0.00	227.80	0.00				
211.55	0.00	228.05	0.00				
212.30	0.00	231.25	1.00				
213.95	0.00	235.05	0.00				

#131: OCTANOIC ACID
Modified: scaled

Entry Number 131 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 65.569
Mol Formula C8H16O2
Mol Weight 144.115

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	149.00	37.00	15.00	47.90	2.00	57.05	1186.00

27.00	2576.00	38.00	57.00	48.15	2.00	58.10	89.00
28.00	623.00	39.00	1423.00	48.50	1.00	59.10	344.00
29.00	3088.00	40.00	258.00	48.85	3.00	60.00	9999.00
30.00	144.00	41.00	4332.00	50.00	31.00	61.00	1267.00
31.00	247.00	42.00	1459.00	50.95	66.00	62.00	73.00
32.95	2.00	43.00	5958.00	52.00	27.00	63.00	16.00
33.35	1.00	44.00	267.00	53.00	229.00	64.00	3.00
33.85	3.00	45.00	1299.00	54.00	126.00	65.00	31.00
35.05	2.00	46.00	40.00	55.00	2803.00	66.00	13.00
36.00	5.00	47.00	36.00	56.10	1048.00	67.05	207.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
68.10	76.00	80.15	32.00	91.15	7.00	103.15	11.00
69.05	1006.00	81.15	38.00	92.10	1.00	104.20	1.00
70.10	170.00	82.15	231.00	93.15	11.00	105.05	3.00
71.10	99.00	83.15	400.00	94.00	2.00	105.70	1.00
73.00	5413.00	84.15	1378.00	95.10	9.00	105.95	1.00
74.05	494.00	85.15	1466.00	96.15	10.00	106.30	1.00
75.05	47.00	86.15	109.00	97.15	131.00	107.15	5.00
76.05	5.00	87.15	991.00	98.15	116.00	108.15	14.00
77.05	14.00	88.15	77.00	99.15	17.00	109.15	4.00
78.05	10.00	89.10	15.00	101.15	1410.00	110.05	1.00
79.05	36.00	90.15	2.00	102.15	103.00	111.10	9.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
112.15	0.00	124.15	5.00	134.30	0.00	142.55	0.00
113.20	3.00	125.10	12.00	135.10	2.00	143.15	2.00
115.15	476.00	126.15	4.00	136.40	0.00	144.15	33.00
116.15	42.00	127.15	39.00	136.65	0.00	145.20	21.00
117.20	5.00	128.15	4.00	136.90	0.00	146.15	2.00
119.00	3.00	129.10	38.00	137.30	0.00	148.10	2.00
120.50	0.00	130.15	3.00	137.90	0.00	148.30	1.00
121.20	1.00	132.15	0.00	139.05	0.00	150.10	1.00
122.10	2.00	132.65	0.00	140.30	0.00	150.90	0.00
123.00	1.00	132.90	0.00	141.30	0.00	151.05	0.00
123.25	1.00	133.25	0.00	142.30	1.00	153.55	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
153.80	0.00	166.05	0.00	187.55	0.00	204.05	0.00
154.55	0.00	167.45	1.00	187.95	0.00	204.70	0.00
155.05	0.00	170.05	1.00	190.05	0.00	207.10	1.00
155.90	0.00	170.30	0.00	191.15	1.00	209.25	1.00
156.90	0.00	170.90	0.00	191.95	0.00	213.20	0.00
157.40	0.00	171.55	0.00	192.20	0.00	213.45	1.00
157.65	1.00	177.90	1.00	193.45	0.00	213.70	0.00
158.30	0.00	179.30	0.00	193.70	0.00	214.10	1.00
162.30	0.00	180.40	0.00	196.95	0.00	218.30	0.00
164.05	1.00	182.05	0.00	198.55	0.00	219.05	1.00
165.05	0.00	185.25	0.00	200.95	0.00	220.30	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
222.70	0.00						

227.30	0.00
229.55	0.00
232.05	0.00
241.45	0.00
242.20	0.00
244.95	0.00

#132: NONANOIC ACID
Modified: scaled

Entry Number 132 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 71.599
Mol Formula C9H18O2
Mol Weight 158.129

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	136.00	35.10	1.00	46.00	37.00	57.10	6661.00
27.00	2573.00	36.00	10.00	47.00	34.00	58.10	328.00
28.00	647.00	37.00	10.00	48.10	5.00	59.10	377.00
29.00	3481.00	38.00	46.00	49.00	2.00	60.00	9999.00
30.00	132.00	39.00	1464.00	50.00	28.00	61.00	1381.00
31.00	228.00	40.00	268.00	51.00	71.00	62.00	71.00
33.00	4.00	41.00	5367.00	52.00	32.00	63.00	15.00
33.10	1.00	42.00	1415.00	53.00	269.00	64.00	1.00
33.90	4.00	43.00	4961.00	54.05	295.00	65.05	42.00
34.35	1.00	44.00	244.00	55.00	3409.00	65.95	18.00
34.75	3.00	45.00	1298.00	56.10	1316.00	67.10	204.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
68.10	192.00	80.10	14.00	91.15	11.00	102.15	54.00
69.05	1380.00	81.15	183.00	92.10	4.00	103.15	7.00
70.10	800.00	82.15	46.00	93.10	32.00	105.15	4.00
71.10	224.00	83.15	593.00	94.15	23.00	106.10	2.00
73.00	6693.00	84.15	352.00	95.15	27.00	107.15	7.00
74.00	573.00	85.15	90.00	96.15	288.00	108.10	2.00
75.00	53.00	86.15	34.00	97.15	229.00	109.00	1.00
76.00	2.00	87.15	998.00	98.15	827.00	109.20	6.00
77.10	24.00	88.15	77.00	99.15	196.00	110.15	3.00
78.10	14.00	89.10	14.00	100.10	22.00	111.15	42.00
79.15	58.00	90.05	1.00	101.15	474.00	112.15	32.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
113.05	5.00	124.15	2.00	131.05	8.00	136.50	1.00
115.15	1499.00	124.25	1.00	132.10	1.00	136.65	0.00
116.15	107.00	124.40	0.00	132.40	1.00	136.85	1.00
117.15	12.00	125.15	5.00	133.15	1.00	137.15	1.00

118.00	1.00	125.95	0.00	134.05	0.00	137.35	1.00
118.20	1.00	126.20	1.00	134.30	0.00	138.10	4.00
119.00	2.00	126.50	0.00	134.55	0.00	139.15	9.00
120.10	1.00	127.00	1.00	135.10	1.00	140.05	1.00
121.10	9.00	127.15	1.00	135.30	0.00	140.30	2.00
122.15	23.00	129.15	1109.00	135.65	0.00	141.15	34.00
123.15	7.00	130.15	93.00	135.95	1.00	142.20	5.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
143.15	7.00	150.00	2.00	158.15	75.00	164.10	1.00
144.30	2.00	151.10	0.00	159.25	21.00	165.30	1.00
145.05	1.00	152.10	1.00	160.05	1.00	167.65	0.00
146.05	0.00	152.30	0.00	160.15	0.00	167.90	0.00
146.15	0.00	152.90	0.00	160.30	1.00	168.25	1.00
146.30	0.00	154.15	2.00	160.55	0.00	169.05	2.00
147.10	1.00	154.55	0.00	160.90	0.00	169.90	1.00
148.35	1.00	155.20	0.00	161.35	1.00	170.15	1.00
148.80	0.00	155.90	0.00	162.90	0.00	170.90	0.00
149.10	1.00	156.15	1.00	163.25	1.00	171.40	0.00
149.30	1.00	157.20	0.00	163.80	0.00	173.40	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
173.80	0.00	185.30	0.00	195.05	0.00	202.20	0.00
174.95	1.00	186.30	0.00	195.45	0.00	207.80	0.00
176.15	0.00	187.45	0.00	195.70	0.00	209.05	0.00
177.20	0.00	188.05	0.00	195.95	0.00	209.30	0.00
178.35	0.00	188.55	0.00	196.20	0.00	209.55	0.00
179.95	0.00	188.80	0.00	196.55	0.00	209.80	0.00
181.05	1.00	189.20	0.00	197.05	0.00	210.05	0.00
181.30	0.00	190.20	0.00	197.70	0.00	211.05	0.00
181.90	0.00	191.20	0.00	198.20	0.00	211.70	0.00
182.15	0.00	193.20	0.00	198.45	0.00	212.40	1.00
183.55	1.00	194.20	0.00	199.45	0.00	213.70	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
214.70	0.00	232.70	0.00				
215.55	0.00	234.95	0.00				
218.05	0.00	235.80	0.00				
220.05	1.00	236.20	0.00				
220.20	1.00	238.00	1.00				
222.70	0.00	239.80	0.00				
226.05	0.00	242.35	0.00				
228.45	0.00						
228.95	0.00						
231.15	1.00						
231.95	0.00						

#133: DECANOIC ACID
Modified: scaled

Entry Number 133 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 78.14
Mol Formula C10H20O2
Mol Weight 172.145

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.10	9.00	37.00	9.00	47.95	4.00	59.10	394.00
26.00	124.00	38.00	25.00	48.95	4.00	60.00	9999.00
27.00	2574.00	39.00	1537.00	50.00	24.00	61.00	1476.00
28.00	585.00	40.00	272.00	51.00	63.00	62.00	74.00
29.00	3948.00	41.00	6036.00	52.05	25.00	63.05	22.00
30.00	130.00	42.00	1593.00	53.00	315.00	65.00	52.00
31.00	246.00	43.00	6301.00	54.05	302.00	66.00	29.00
33.00	3.00	44.00	242.00	55.00	4151.00	67.05	267.00
33.95	0.00	45.00	1270.00	56.10	1099.00	68.10	326.00
35.10	1.00	46.00	33.00	57.10	4928.00	69.05	1575.00
36.00	7.00	47.00	31.00	58.05	256.00	70.10	874.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
71.10	3634.00	83.15	1235.00	94.15	31.00	105.10	6.00
73.00	7638.00	84.15	761.00	95.15	73.00	106.05	0.00
74.00	676.00	85.15	125.00	96.15	39.00	107.15	28.00
75.05	61.00	86.15	58.00	97.15	340.00	108.15	9.00
75.95	11.00	87.15	1370.00	98.15	259.00	109.15	13.00
77.05	30.00	88.15	118.00	99.15	43.00	110.15	275.00
78.15	18.00	89.15	20.00	100.05	11.00	111.15	94.00
79.10	82.00	90.10	1.00	101.15	461.00	112.15	380.00
80.10	28.00	91.15	15.00	102.15	57.00	113.15	89.00
81.15	211.00	92.10	3.00	103.05	8.00	114.25	16.00
82.15	318.00	93.15	37.00	104.15	1.00	115.15	824.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
116.15	64.00	127.05	4.00	137.25	5.00	146.05	1.00
117.10	10.00	129.15	2427.00	138.20	3.00	146.30	1.00
119.00	3.00	130.15	186.00	139.15	5.00	148.25	1.00
119.75	1.00	131.05	20.00	139.90	1.00	148.55	1.00
120.40	1.00	132.10	3.00	140.15	1.00	149.05	1.00
121.10	14.00	132.80	1.00	141.20	1.00	150.05	1.00
122.15	3.00	133.05	0.00	141.55	1.00	152.20	2.00
123.10	7.00	133.40	1.00	141.80	1.00	153.20	7.00
124.10	3.00	133.80	1.00	143.15	416.00	154.15	3.00
125.10	19.00	135.10	15.00	144.20	41.00	155.20	32.00
126.15	6.00	136.20	27.00	145.15	6.00	156.15	2.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
156.40	1.00	167.55	1.00	179.40	0.00	201.45	0.00
157.25	7.00	167.80	1.00	181.15	2.00	202.45	0.00
158.25	4.00	169.05	1.00	181.90	1.00	203.20	0.00

159.00	0.00	172.20	145.00	184.90	0.00	205.05	1.00
159.80	0.00	173.25	30.00	188.30	0.00	205.70	0.00
160.30	1.00	174.30	4.00	192.30	0.00	207.40	1.00
161.05	0.00	175.05	1.00	194.30	1.00	210.55	0.00
163.05	1.00	175.90	1.00	194.55	1.00	212.30	0.00
164.05	2.00	176.90	0.00	197.20	0.00	212.80	0.00
166.05	1.00	177.30	0.00	197.95	1.00	215.20	0.00
166.40	0.00	178.30	1.00	198.30	1.00	216.55	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
217.30	1.00						
220.05	2.00						
222.20	0.00						
232.70	1.00						
234.80	0.00						
236.55	1.00						
242.95	0.00						
245.35	0.00						

#134: 5-METHYL-2-HEXANONE
Modified: scaled

Entry Number 134 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 34.57
Mol Formula C7H14O
Mol Weight 114.103

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.10	1.00	35.80	1.00	47.00	1.00	58.00	4111.00
26.00	81.00	37.00	15.00	48.00	6.00	59.00	1086.00
27.00	925.00	38.00	44.00	48.95	4.00	60.00	40.00
28.00	217.00	39.00	615.00	50.00	28.00	61.00	4.00
29.00	739.00	40.00	93.00	51.00	43.00	62.00	3.00
29.95	24.00	40.95	1307.00	52.00	16.00	63.05	5.00
31.00	42.00	42.10	369.00	53.00	114.00	64.00	1.00
32.90	1.00	43.00	9999.00	54.05	34.00	65.05	9.00
33.35	0.00	44.00	282.00	55.00	359.00	66.00	3.00
34.00	2.00	45.00	62.00	56.10	320.00	67.05	18.00
35.00	1.00	46.00	1.00	57.05	1415.00	68.00	3.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
69.00	21.00	79.15	18.00	90.30	0.00	98.15	1.00
70.10	54.00	81.15	406.00	91.10	1.00	99.15	90.00
71.00	790.00	82.15	27.00	92.15	0.00	100.10	5.00
72.10	93.00	83.05	5.00	92.40	0.00	101.05	0.00
73.10	8.00	85.10	163.00	93.15	1.00	102.15	0.00

74.10	1.00	86.15	135.00	93.90	0.00	103.05	0.00
75.05	1.00	87.15	8.00	94.15	0.00	103.40	0.00
75.60	0.00	88.00	0.00	95.15	18.00	104.15	0.00
75.90	0.00	89.15	0.00	96.00	1.00	104.75	0.00
77.10	7.00	89.40	0.00	96.20	2.00	105.45	0.00
78.10	1.00	89.75	0.00	97.15	12.00	106.20	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
108.00	0.00	113.15	1.00	120.90	0.00	126.90	0.00
108.50	0.00	114.15	178.00	121.15	0.00	127.65	0.00
108.90	0.00	115.15	34.00	121.50	0.00	127.90	0.00
109.20	0.00	116.15	3.00	121.75	0.00	128.20	0.00
109.65	0.00	117.25	0.00	122.90	0.00	128.90	0.00
109.75	0.00	117.60	0.00	123.15	0.00	129.25	0.00
109.90	0.00	118.00	0.00	123.40	0.00	130.25	0.00
110.20	0.00	118.25	0.00	125.00	0.00	132.00	0.00
110.75	0.00	119.00	0.00	125.40	0.00	132.30	0.00
111.40	0.00	119.75	0.00	126.00	0.00	136.20	0.00
112.10	1.00	120.00	0.00	126.65	0.00	137.30	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
137.55	0.00	149.00	0.00	158.30	0.00	169.05	0.00
138.15	0.00	149.80	0.00	159.15	0.00	169.90	0.00
139.90	0.00	151.10	0.00	161.30	0.00	170.65	0.00
140.80	0.00	151.65	0.00	162.15	0.00	171.05	0.00
141.10	0.00	152.80	0.00	163.40	0.00	172.15	0.00
143.90	0.00	153.15	0.00	164.30	0.00	173.25	0.00
144.15	0.00	154.40	0.00	164.80	0.00	174.65	0.00
145.65	0.00	154.80	0.00	165.80	0.00	175.15	0.00
147.10	0.00	155.85	0.00	166.40	0.00	176.20	0.00
147.30	0.00	156.65	0.00	167.80	0.00	179.65	0.00
147.80	0.00	157.65	0.00	168.40	0.00	180.05	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
181.05	0.00	192.30	0.00	210.55	0.00	236.55	0.00
181.65	0.00	193.20	0.00	210.80	0.00	237.30	0.00
183.05	0.00	193.55	0.00	215.20	0.00	239.45	0.00
183.65	0.00	196.55	0.00	219.05	1.00	241.95	0.00
183.90	0.00	198.20	0.00	219.95	0.00	246.85	0.00
184.80	0.00	200.00	0.00	221.80	0.00	248.10	0.00
187.05	0.00	203.30	0.00	223.30	0.00		
188.20	0.00	204.20	0.00	225.95	0.00		
189.55	0.00	207.05	0.00	227.95	0.00		
191.30	0.00	208.95	0.00	233.45	0.00		
191.80	0.00	210.30	0.00	234.95	0.00		

#135: CYCLOHEXANONE
Modified: scaled

Entry Number 135 from C:\DATABASE\hjf.l

CAS	000000-00-0
Melting Point	-300
Boiling Point	-300
Retention Index	39.469
Mol Formula	C6H10O
Mol Weight	98.072

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	435.00	37.00	104.00	47.00	2.00	58.00	11.00
27.00	2457.00	38.00	243.00	48.00	7.00	59.05	0.00
28.00	1014.00	39.00	2371.00	49.00	20.00	60.00	2.00
29.00	889.00	40.00	636.00	50.00	126.00	61.00	15.00
29.95	20.00	41.00	3434.00	51.00	150.00	62.00	25.00
31.00	60.00	42.00	7793.00	51.95	57.00	63.00	31.00
32.00	14.00	43.00	1427.00	53.00	272.00	64.00	5.00
33.00	22.00	44.00	100.00	54.05	789.00	65.00	39.00
34.00	30.00	45.00	6.00	55.00	9999.00	66.00	18.00
34.95	5.00	45.85	1.00	56.00	1288.00	67.05	69.00
36.05	5.00	46.00	0.00	57.00	140.00	68.10	80.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
69.00	2723.00	80.15	421.00	90.00	0.00	97.15	185.00
70.00	1950.00	81.10	36.00	90.50	0.00	98.15	2908.00
71.05	146.00	83.15	666.00	90.85	0.00	99.15	213.00
72.05	4.00	84.15	38.00	91.65	0.00	100.10	13.00
73.00	3.00	85.00	2.00	91.90	0.00	101.00	1.00
74.05	7.00	86.15	0.00	92.20	0.00	101.75	0.00
75.00	2.00	86.95	1.00	93.15	0.00	102.00	0.00
76.00	1.00	87.25	0.00	94.00	1.00	103.15	0.00
77.00	13.00	87.65	0.00	94.15	1.00	103.50	0.00
78.15	3.00	88.05	0.00	95.10	1.00	106.90	0.00
79.15	100.00	88.40	0.00	96.15	2.00	107.40	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
107.65	0.00	120.75	0.00	128.40	0.00	141.10	0.00
108.25	0.00	122.25	0.00	128.65	0.00	142.10	0.00
110.10	0.00	123.25	0.00	131.00	0.00	144.15	0.00
111.75	0.00	124.75	0.00	133.30	0.00	145.15	0.00
112.95	0.00	125.10	0.00	134.15	0.00	145.35	0.00
115.20	0.00	125.90	0.00	134.80	0.00	146.05	0.00
115.90	0.00	126.25	0.00	135.05	0.00	146.30	0.00
116.40	0.00	126.65	0.00	137.80	0.00	147.05	1.00
116.65	0.00	127.40	0.00	138.30	0.00	148.15	0.00
118.00	0.00	127.65	0.00	139.05	0.00	149.40	0.00
119.00	0.00	127.95	0.00	140.40	0.00	149.90	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
151.00	0.00	164.80	0.00	185.55	0.00	205.20	0.00
154.05	0.00	165.80	0.00	187.05	0.00	205.70	0.00
154.40	0.00	166.05	0.00	187.45	0.00	205.95	0.00
155.05	0.00	166.90	0.00	188.20	0.00	213.05	0.00

155.90	0.00	170.15	0.00	190.55	0.00	214.20	0.00
160.40	0.00	171.05	0.00	193.20	0.00	219.05	0.00
160.80	0.00	175.90	0.00	194.30	0.00	220.05	0.00
161.30	0.00	176.15	0.00	195.20	0.00	221.95	0.00
162.15	0.00	178.15	0.00	196.95	0.00	232.55	0.00
164.15	0.00	178.80	0.00	197.55	0.00	233.80	0.00
164.40	0.00	184.65	0.00	199.55	0.00	248.45	0.00

#136: 2-METHYLCYCLOHEXANONE
Modified: scaled

Entry Number 136 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 43.049
Mol Formula C7H12O
Mol Weight 112.088

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	503.00	37.00	75.00	47.00	1.00	58.00	404.00
27.00	3724.00	37.95	248.00	47.75	1.00	59.05	13.00
28.00	2149.00	39.00	3540.00	49.00	17.00	60.05	3.00
29.00	1904.00	39.95	1008.00	49.95	170.00	61.00	14.00
29.95	51.00	41.00	8869.00	51.00	262.00	61.95	27.00
31.00	38.00	42.00	5577.00	52.00	109.00	62.95	48.00
32.80	6.00	43.00	2286.00	53.00	644.00	63.95	8.00
33.00	9.00	44.00	53.00	54.10	411.00	65.00	92.00
33.95	10.00	45.00	21.00	55.00	7505.00	66.00	52.00
34.75	1.00	46.00	3.00	56.10	6429.00	67.05	1272.00
36.05	2.00	46.35	0.00	57.00	578.00	68.05	9999.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
69.00	5452.00	80.15	26.00	89.05	1.00	100.00	0.00
70.00	1104.00	81.10	63.00	89.90	1.00	101.25	0.00
71.05	148.00	82.10	18.00	90.40	0.00	101.65	0.00
72.05	8.00	83.15	1228.00	91.00	11.00	102.80	0.00
73.00	4.00	84.10	2306.00	92.15	2.00	103.40	0.00
74.00	10.00	85.10	134.00	93.10	15.00	103.65	0.00
75.05	4.00	86.05	8.00	94.10	254.00	105.50	0.00
76.00	2.00	87.00	1.00	95.15	34.00	105.75	0.00
77.00	54.00	87.40	0.00	97.10	711.00	106.05	0.00
78.15	26.00	87.80	1.00	98.15	45.00	107.15	1.00
79.15	368.00	88.40	0.00	99.15	3.00	108.10	2.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
109.15	1.00	122.20	0.00	129.00	0.00	137.05	0.00
110.10	10.00	123.00	0.00	129.15	0.00	139.35	0.00
112.10	3863.00	123.20	0.00	129.40	0.00	141.55	0.00

113.10	329.00	123.70	1.00	132.90	0.00	142.70	0.00
114.10	19.00	124.90	0.00	133.30	0.00	143.30	0.00
115.20	1.00	125.15	0.00	133.65	0.00	143.70	0.00
117.40	0.00	125.40	0.00	134.40	0.00	144.85	0.00
117.65	0.00	126.15	0.00	135.80	0.00	148.65	0.00
119.00	0.00	126.90	0.00	136.05	0.00	150.55	0.00
120.25	0.00	127.65	0.00	136.40	0.00	150.90	1.00
121.90	0.00	127.95	0.00	136.80	0.00	151.90	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
153.30	0.00	171.10	0.00	207.05	0.00	236.30	0.00
155.35	0.00	173.90	0.00	207.70	0.00	237.95	0.00
155.65	0.00	176.40	0.00	214.05	0.00	238.55	0.00
157.90	0.00	181.15	0.00	215.20	0.00	240.95	0.00
158.15	0.00	181.40	0.00	217.45	0.00	242.00	0.00
159.65	0.00	182.65	0.00	217.95	0.00		
160.40	0.00	185.05	0.00	219.80	0.00		
161.70	0.00	188.70	0.00	220.35	0.00		
162.90	0.00	193.05	0.00	227.30	0.00		
169.00	1.00	199.70	0.00	229.70	0.00		
170.40	0.00	201.20	0.00	233.70	0.00		

#137: 1,2-EPOXYOCTANE
Modified: scaled

Entry Number 137 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 44.609
Mol Formula C8H16O
Mol Weight 128.12

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	266.00	37.00	28.00	47.75	0.00	58.00	4802.00
27.00	4169.00	38.00	117.00	48.00	1.00	59.00	535.00
28.00	1016.00	38.95	2973.00	49.00	2.00	60.05	21.00
29.00	6826.00	40.00	572.00	49.95	60.00	60.85	2.00
30.00	273.00	41.00	9999.00	51.00	133.00	61.05	2.00
31.00	1783.00	42.00	5089.00	52.00	60.00	62.05	9.00
32.95	15.00	43.00	4743.00	53.00	620.00	63.00	19.00
34.00	1.00	44.00	686.00	54.00	1193.00	63.95	5.00
34.30	2.00	45.00	940.00	55.05	6095.00	65.00	89.00
35.00	0.00	45.95	20.00	56.05	3929.00	66.05	103.00
36.05	1.00	47.00	2.00	57.05	2340.00	67.05	1412.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
68.05	2049.00	79.15	133.00	89.65	0.00	101.15	4.00
69.05	2372.00	81.10	2116.00	91.10	9.00	102.75	0.00

70.10	2133.00	82.10	346.00	92.25	1.00	103.25	0.00
71.05	8929.00	83.10	234.00	93.10	14.00	104.00	0.00
72.10	581.00	84.10	127.00	94.25	1.00	104.25	0.00
73.05	61.00	85.10	1211.00	95.10	190.00	104.80	0.00
73.95	5.00	86.10	106.00	96.10	201.00	105.15	1.00
75.00	1.00	87.10	14.00	97.10	98.00	106.25	1.00
76.05	1.00	87.90	0.00	98.15	33.00	107.20	2.00
77.00	36.00	88.15	1.00	99.15	328.00	107.90	0.00
78.10	8.00	88.75	0.00	100.10	51.00	109.15	10.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
110.15	18.00	120.00	0.00	128.20	3.00	143.05	0.00
111.05	4.00	120.95	1.00	128.95	1.00	144.40	0.00
112.20	5.00	123.20	0.00	129.15	1.00	145.05	0.00
113.15	18.00	123.75	0.00	130.25	0.00	145.40	0.00
114.05	1.00	124.10	1.00	131.90	0.00	146.90	1.00
115.90	0.00	124.50	1.00	133.15	0.00	148.80	0.00
116.15	0.00	124.90	0.00	134.40	0.00	150.40	1.00
117.00	0.00	125.20	1.00	137.15	0.00	157.15	0.00
117.25	0.00	125.90	0.00	139.30	0.00	157.90	0.00
117.55	0.00	127.15	11.00	140.90	1.00	158.55	0.00
117.90	0.00	128.00	1.00	141.20	0.00	159.55	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
159.90	0.00	183.80	0.00	238.20	0.00		
164.05	0.00	185.05	0.00	239.95	0.00		
164.30	0.00	194.70	0.00	244.85	0.00		
165.05	0.00	195.30	0.00	245.55	0.00		
166.55	0.00	197.45	0.00				
166.80	0.00	210.30	0.00				
171.10	0.00	215.05	0.00				
181.05	0.00	222.20	0.00				
182.10	0.00	224.10	0.00				
183.30	0.00	225.80	0.00				
183.55	0.00	230.95	0.00				

#138: 2-HEXANONE
Modified: scaled

Entry Number 138 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 28.55
Mol Formula C6H12O
Mol Weight 100.088

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.10	4.00	34.95	1.00	45.95	1.00	58.00	4367.00

26.00	160.00	36.00	2.00	46.95	2.00	59.00	256.00
27.00	1123.00	37.00	21.00	49.00	6.00	60.05	14.00
28.00	311.00	38.00	58.00	50.00	38.00	61.10	2.00
29.00	1976.00	38.95	612.00	50.95	43.00	61.95	3.00
30.00	56.00	39.95	83.00	52.00	13.00	63.00	3.00
31.00	46.00	41.00	1640.00	53.00	72.00	63.90	1.00
32.90	0.00	42.00	451.00	54.00	19.00	65.05	5.00
34.10	1.00	43.00	9999.00	54.95	157.00	65.95	2.00
34.35	0.00	44.00	215.00	56.05	66.00	67.05	13.00
34.70	1.00	45.00	60.00	57.10	1409.00	67.95	2.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
69.00	3.00	79.05	3.00	88.65	0.00	96.00	0.00
71.10	388.00	80.40	0.00	89.75	0.00	96.90	0.00
72.10	99.00	81.05	1.00	90.75	0.00	97.15	1.00
73.00	5.00	82.05	1.00	91.20	0.00	98.15	2.00
74.00	1.00	82.25	0.00	91.45	1.00	100.10	558.00
74.85	0.00	83.10	7.00	92.05	0.00	101.10	47.00
75.10	1.00	85.10	583.00	92.25	0.00	102.20	3.00
76.00	1.00	86.10	33.00	92.40	0.00	103.90	0.00
77.00	4.00	87.05	1.00	92.70	0.00	105.15	0.00
77.70	0.00	87.90	1.00	94.90	0.00	105.65	0.00
78.15	0.00	88.40	0.00	95.00	0.00	106.40	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
106.70	0.00	114.00	0.00	123.25	0.00	136.55	0.00
108.00	0.00	115.20	0.00	124.25	0.00	136.80	0.00
108.40	0.00	116.15	0.00	124.85	0.00	137.30	0.00
108.90	0.00	116.25	0.00	129.00	0.00	140.30	0.00
109.15	0.00	116.40	0.00	130.25	0.00	140.55	0.00
109.35	0.00	117.90	0.00	133.25	0.00	140.80	0.00
109.65	0.00	119.00	1.00	134.80	0.00	141.40	0.00
110.20	0.00	120.15	1.00	135.05	0.00	143.00	0.00
111.40	0.00	120.50	0.00	135.40	0.00	144.50	0.00
111.75	0.00	121.00	0.00	135.65	0.00	144.90	0.00
112.15	0.00	123.00	0.00	136.30	0.00	147.05	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
150.40	0.00	164.05	0.00	181.20	0.00	200.70	0.00
150.65	0.00	165.40	0.00	182.80	0.00	201.05	0.00
151.00	0.00	167.80	0.00	185.05	0.00	202.80	0.00
153.65	0.00	169.00	1.00	185.40	0.00	203.95	0.00
154.30	0.00	169.85	0.00	187.20	0.00	205.80	0.00
154.80	0.00	171.80	0.00	187.45	0.00	207.20	0.00
158.55	0.00	173.05	0.00	188.70	0.00	213.05	0.00
161.40	0.00	176.05	0.00	188.95	0.00	214.05	0.00
161.90	0.00	176.40	0.00	191.80	0.00	219.95	0.00
163.05	0.00	178.55	0.00	195.95	0.00	220.20	0.00
163.30	0.00	180.90	0.00	200.45	0.00	220.55	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
224.95	0.00						

228.05	0.00
228.70	0.00
231.05	0.00
232.95	0.00
238.30	0.00
246.20	0.00

#139: DIHYDRO-2(3H)-FURANONE
Modified: scaled

Entry Number 139 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 48.89
Mol Formula C4H6O2
Mol Weight 86.037
Miscellaneous Information
Aldrich: gamma-butyrolactone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	1595.00	36.95	226.00	49.00	5.00	62.25	2.00
27.00	3852.00	38.00	318.00	50.00	2.00	65.00	2.00
28.00	9999.00	39.00	1123.00	52.10	11.00	66.75	3.00
29.00	5515.00	40.00	831.00	53.00	81.00	67.10	2.00
29.95	304.00	41.00	3342.00	53.95	40.00	68.00	6.00
31.00	269.00	42.00	7858.00	55.00	576.00	69.00	7.00
32.00	14.00	43.00	458.00	56.00	2103.00	70.00	6.00
33.00	8.00	44.00	110.00	57.00	505.00	71.10	0.00
34.00	6.00	45.00	45.00	58.00	19.00	72.75	3.00
34.75	3.00	46.05	1.00	59.25	6.00	74.25	1.00
35.95	35.00	47.75	3.00	60.85	2.00	74.60	2.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
74.85	2.00	88.10	6.00	101.00	0.00	115.00	2.00
75.90	1.00	89.40	2.00	101.75	2.00	119.00	4.00
77.05	2.00	90.15	2.00	103.15	0.00	119.95	0.00
77.90	3.00	91.25	3.00	103.40	2.00	125.15	1.00
80.40	1.00	91.75	2.00	106.00	1.00	128.15	1.00
82.05	2.00	93.15	3.00	106.75	2.00	131.00	4.00
83.25	7.00	94.20	1.00	107.95	0.00	132.15	2.00
84.00	3.00	95.25	0.00	110.15	1.00	134.30	1.00
85.00	519.00	96.15	1.00	112.25	0.00	137.40	2.00
86.15	1973.00	97.05	2.00	112.90	2.00	139.05	2.00
87.15	90.00	99.15	1.00	114.75	2.00	142.55	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
144.90	2.00	219.05	2.00				
148.65	1.00	220.20	2.00				

150.15	0.00
151.30	1.00
157.30	1.00
163.90	1.00
169.05	2.00
171.80	1.00
172.05	2.00
189.20	1.00
198.45	2.00

#140: 4-METHYLCYCLOHEXANONE
Modified: scaled

Entry Number 140 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 44.689
Mol Formula C7H12O
Mol Weight 112.088

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	350.00	39.00	1898.00	51.00	205.00	63.00	29.00
27.00	2487.00	40.00	423.00	52.00	85.00	64.05	4.00
28.00	1612.00	41.00	4804.00	53.00	463.00	65.00	55.00
29.00	1911.00	42.00	2217.00	55.00	9999.00	66.10	28.00
30.00	45.00	43.00	893.00	56.05	4103.00	67.05	315.00
31.00	28.00	44.00	4.00	57.05	1766.00	68.05	519.00
33.00	15.00	45.05	5.00	58.00	104.00	69.05	1114.00
33.85	11.00	46.90	0.00	59.10	2.00	70.10	1425.00
35.95	2.00	48.00	4.00	60.00	1.00	71.05	76.00
36.95	42.00	48.95	13.00	61.00	10.00	72.10	4.00
38.00	142.00	50.00	132.00	62.00	19.00	72.90	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
73.95	4.00	87.15	1.00	102.40	0.00	112.15	2171.00
75.10	2.00	89.15	1.00	102.65	0.00	113.15	196.00
77.00	31.00	91.15	6.00	103.40	0.00	114.10	11.00
78.10	37.00	92.00	1.00	104.40	0.00	115.15	1.00
79.10	646.00	93.15	18.00	105.15	0.00	118.15	0.00
80.15	46.00	94.15	416.00	106.40	1.00	119.80	0.00
81.15	26.00	95.15	40.00	107.00	0.00	121.00	0.00
83.15	2040.00	97.15	385.00	107.25	0.00	123.50	0.00
84.10	1115.00	98.15	26.00	107.90	1.00	123.75	0.00
85.15	79.00	99.05	0.00	109.15	1.00	125.15	0.00
86.15	3.00	101.20	0.00	110.15	3.00	128.50	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
129.00	0.00	166.05	1.00				

129.25	0.00	169.05	0.00
131.00	0.00	173.05	1.00
132.55	0.00	191.80	0.00
142.15	0.00	194.05	0.00
143.15	0.00	207.20	0.00
146.15	0.00	210.20	0.00
147.05	0.00	214.05	0.00
153.15	1.00	226.20	1.00
158.65	0.00		
162.55	0.00		

#141: 3-METHYLCYCLOHEXANOL
Modified: scaled

Entry Number 141 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 43.49
Mol Formula C7H14O
Mol Weight 114.103

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	180.00	38.00	134.00	49.00	9.00	59.95	6.00
27.00	2753.00	39.00	2456.00	50.00	89.00	61.00	6.00
28.00	424.00	40.00	458.00	51.00	196.00	62.00	12.00
29.00	3172.00	41.00	4967.00	52.00	80.00	63.00	31.00
30.00	155.00	42.00	3059.00	53.00	811.00	63.95	8.00
31.00	966.00	43.00	4265.00	54.00	1076.00	65.05	118.00
33.00	7.00	44.00	3125.00	55.10	4214.00	65.95	247.00
33.90	3.00	45.00	501.00	56.10	1032.00	67.10	1492.00
34.80	8.00	46.10	22.00	57.00	5373.00	68.10	1343.00
35.95	4.00	47.10	23.00	58.00	554.00	69.05	823.00
37.00	40.00	48.00	21.00	59.10	140.00	70.10	1186.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
71.00	9999.00	83.10	110.00	94.25	22.00	103.65	2.00
72.10	584.00	84.10	30.00	95.15	565.00	105.00	1.00
73.10	52.00	85.15	70.00	96.15	3665.00	105.90	1.00
74.00	8.00	86.10	177.00	97.15	337.00	107.25	2.00
75.00	4.00	87.10	10.00	98.15	14.00	108.95	1.00
76.00	2.00	88.00	3.00	99.15	172.00	110.15	3.00
77.15	94.00	89.00	2.00	100.10	13.00	110.90	1.00
78.15	15.00	89.65	3.00	101.15	1.00	111.15	1.00
79.15	315.00	91.15	34.00	102.15	1.00	112.15	32.00
81.15	7170.00	92.15	6.00	102.40	1.00	113.15	114.00
82.15	483.00	93.15	38.00	102.75	1.00	114.10	45.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.

115.10	5.00	142.15	1.00	197.20	1.00
116.50	1.00	145.05	2.00	209.45	1.00
119.00	1.00	150.05	1.00	224.95	1.00
124.25	1.00	154.15	1.00	230.55	1.00
127.15	1.00	157.80	2.00		
127.40	1.00	176.05	1.00		
128.00	2.00	179.30	1.00		
129.15	1.00	180.90	1.00		
131.00	1.00	185.80	1.00		
135.40	2.00	187.05	2.00		
138.40	1.00	187.30	1.00		

#142: 2-METHYLCYCLOPENTANONE
Modified: scaled

Entry Number 142 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 33.929
Mol Formula C6H10O
Mol Weight 98.072

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.10	17.00	36.05	6.00	46.95	3.00	58.05	14.00
25.95	491.00	37.00	100.00	48.00	4.00	58.85	0.00
27.00	2446.00	38.00	233.00	48.95	22.00	59.10	1.00
28.00	2070.00	39.00	2255.00	49.95	110.00	60.00	4.00
29.00	1071.00	40.00	630.00	51.00	147.00	61.00	17.00
29.95	24.00	41.00	4077.00	51.95	61.00	61.95	22.00
30.95	71.00	42.00	9999.00	53.00	332.00	63.00	32.00
32.00	6.00	43.00	1486.00	54.00	447.00	64.00	5.00
32.95	23.00	44.00	39.00	55.00	5391.00	65.00	42.00
33.95	24.00	45.00	6.00	56.00	1889.00	66.00	16.00
35.10	1.00	46.25	1.00	56.95	165.00	67.10	92.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
69.00	2781.00	80.10	284.00	91.75	0.00	100.10	13.00
70.05	1533.00	81.10	34.00	92.00	0.00	101.00	1.00
71.05	95.00	83.10	725.00	92.20	0.00	101.90	0.00
72.00	5.00	84.10	41.00	92.50	0.00	102.65	0.00
73.05	1.00	85.10	3.00	93.15	0.00	103.40	0.00
74.05	4.00	87.15	0.00	94.00	2.00	104.90	0.00
75.00	1.00	87.65	0.00	95.10	3.00	105.00	0.00
76.05	1.00	87.95	0.00	96.15	10.00	105.15	0.00
77.05	10.00	89.90	0.00	97.15	169.00	105.50	0.00
78.10	1.00	90.15	0.00	98.10	2887.00	108.00	0.00
79.10	125.00	90.85	0.00	99.15	201.00	108.70	1.00

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
109.00	0.00	122.90	0.00	135.55	0.00	157.30	0.00
111.15	0.00	125.70	0.00	137.90	0.00	164.05	0.00
113.00	0.00	127.00	0.00	138.90	0.00	167.15	0.00
114.00	0.00	127.40	0.00	143.20	0.00	169.10	0.00
115.00	0.00	127.65	0.00	143.55	0.00	171.15	0.00
116.15	0.00	127.90	0.00	148.80	0.00	171.40	0.00
117.90	0.00	128.90	0.00	149.40	0.00	171.65	0.00
118.15	0.00	129.25	0.00	150.90	0.00	181.00	0.00
119.00	1.00	132.15	0.00	151.15	0.00	182.05	0.00
122.00	0.00	132.30	0.00	151.90	0.00	193.30	0.00
122.25	0.00	133.40	0.00	152.40	0.00	200.70	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
210.80	0.00						
212.45	0.00						
215.20	0.00						
221.55	0.00						

#143: HEXANOL
Modified: scaled

Entry Number 143 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 37.289
Mol Formula C6H14O
Mol Weight 102.103
Miscellaneous Information
Aldrich: hexyl alcohol

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	162.00	36.95	23.00	47.75	0.00	58.10	30.00
27.00	2266.00	37.95	74.00	48.00	1.00	59.00	33.00
28.00	569.00	39.00	1263.00	49.00	3.00	60.10	3.00
29.00	3145.00	40.05	294.00	50.00	35.00	61.00	3.00
30.05	127.00	41.00	4890.00	51.00	54.00	61.95	5.00
31.00	3325.00	42.00	4636.00	51.95	21.00	63.05	6.00
32.00	26.00	43.00	6428.00	53.00	203.00	63.95	2.00
33.00	38.00	44.00	433.00	54.10	279.00	65.05	20.00
34.00	1.00	45.00	296.00	55.00	4584.00	66.05	5.00
34.80	2.00	45.95	18.00	56.10	9999.00	67.10	85.00
35.85	1.00	46.95	3.00	57.05	765.00	68.05	77.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
69.05	2628.00	79.10	6.00	89.15	0.00	98.05	1.00
70.05	222.00	80.00	1.00	91.00	0.00	99.20	0.00
71.05	115.00	81.10	6.00	92.15	0.00	100.05	0.00

72.10	29.00	82.10	11.00	93.25	0.00	101.10	5.00
73.10	88.00	83.10	84.00	93.90	0.00	102.10	0.00
74.10	6.00	84.10	337.00	95.15	0.00	103.20	1.00
75.05	1.00	85.10	34.00	95.50	0.00	106.65	0.00
76.15	0.00	86.10	2.00	95.75	0.00	106.90	0.00
77.10	4.00	87.20	0.00	96.20	0.00	107.95	1.00
77.90	1.00	87.50	0.00	97.00	1.00	109.00	0.00
78.10	1.00	88.25	0.00	97.20	0.00	109.25	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
109.50	0.00	139.55	0.00	161.40	0.00	201.95	0.00
115.50	0.00	142.90	0.00	161.80	0.00	202.20	0.00
116.15	1.00	144.95	0.00	162.65	0.00	207.05	0.00
117.65	0.00	148.40	0.00	164.15	0.00	219.05	0.00
120.00	0.00	148.65	0.00	167.30	0.00	220.05	0.00
121.50	0.00	150.10	0.00	170.90	0.00	224.30	0.00
124.00	0.00	150.35	0.00	175.90	0.00	224.95	0.00
127.00	0.00	154.05	0.00	188.30	0.00	232.20	0.00
128.15	0.00	155.30	0.00	192.80	0.00	234.55	0.00
128.40	0.00	156.15	0.00	193.05	0.00		
129.75	0.00	156.55	0.00	197.80	0.00		

#144: TETRAHYDRO-3-FURANOL
Modified: scaled

Entry Number 144 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 40.75
Mol Formula C4H8O2
Mol Weight 88.052
Miscellaneous Information
Aldrich: 3-hydroxytetrahydrofuran

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.10	6.00	34.25	1.00	44.00	1680.00	54.00	11.00
26.00	476.00	34.60	1.00	45.00	594.00	55.00	185.00
27.00	1759.00	35.10	2.00	46.05	15.00	56.05	73.00
28.00	2437.00	36.00	11.00	47.00	60.00	57.00	9999.00
29.00	5542.00	36.95	98.00	48.00	2.00	58.00	7517.00
30.00	2890.00	38.00	183.00	48.30	2.00	59.00	404.00
31.00	5757.00	39.00	1337.00	49.00	6.00	60.05	784.00
32.00	1190.00	40.00	937.00	49.95	14.00	60.95	86.00
33.00	167.00	41.00	1128.00	51.00	10.00	62.00	2.00
34.00	3.00	42.00	1220.00	52.00	5.00	62.10	1.00
34.10	2.00	43.00	2178.00	53.00	29.00	62.25	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.

63.05	0.00	72.05	6.00	79.15	1.00	90.10	5.00
63.75	1.00	73.05	11.00	79.60	0.00	91.00	1.00
64.50	1.00	74.00	0.00	80.40	0.00	92.00	1.00
65.15	2.00	74.75	0.00	81.95	1.00	93.15	0.00
66.00	0.00	75.30	1.00	83.10	1.00	93.40	0.00
66.85	1.00	75.85	1.00	83.95	1.00	94.25	1.00
67.10	1.00	76.35	1.00	85.05	2.00	95.15	1.00
68.00	14.00	77.20	1.00	86.05	18.00	95.90	0.00
69.00	78.00	77.75	1.00	87.10	67.00	96.95	1.00
70.00	1450.00	78.00	1.00	88.15	969.00	98.45	0.00
71.05	89.00	78.65	0.00	89.15	47.00	100.00	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
101.00	2.00	109.50	0.00	119.00	0.00	129.40	1.00
102.40	0.00	110.25	0.00	121.65	0.00	129.50	0.00
103.40	0.00	110.75	0.00	121.95	1.00	131.05	2.00
103.65	0.00	111.40	1.00	122.75	0.00	131.80	0.00
103.90	1.00	112.20	0.00	123.15	0.00	132.10	0.00
104.90	1.00	112.90	0.00	123.50	0.00	133.05	0.00
105.75	0.00	114.20	1.00	123.90	0.00	133.65	0.00
106.50	0.00	115.25	0.00	124.20	0.00	135.60	0.00
107.00	0.00	115.65	0.00	126.15	0.00	138.90	0.00
108.15	0.00	116.05	0.00	128.70	0.00	139.30	0.00
108.55	0.00	116.65	0.00	129.00	0.00	139.80	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
141.15	0.00	150.40	0.00	172.40	0.00	202.55	0.00
143.15	1.00	151.05	0.00	173.40	0.00	204.55	0.00
143.30	0.00	155.15	0.00	176.40	0.00	206.55	0.00
144.55	0.00	155.40	0.00	182.80	0.00	207.30	0.00
144.90	0.00	158.65	0.00	184.80	0.00	211.95	0.00
146.85	1.00	160.15	0.00	187.95	0.00	220.00	0.00
147.40	0.00	162.90	0.00	188.70	0.00	240.60	0.00
147.65	0.00	166.30	0.00	188.95	0.00		
148.05	0.00	166.90	0.00	190.30	0.00		
149.40	0.00	169.05	0.00	201.45	0.00		
149.65	0.00	170.40	0.00	201.95	0.00		

#145: 2-METHYLCYCLOHEXANOL
Modified: scaled

Entry Number 145 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 42.49
Mol Formula C7H14O
Mol Weight 114.103

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.10	6.00	37.00	38.00	47.95	8.00	59.00	121.00
26.00	226.00	38.00	137.00	49.00	8.00	60.10	9.00
27.00	2828.00	39.00	2426.00	50.00	93.00	61.00	5.00
28.00	718.00	40.00	480.00	50.95	211.00	62.00	14.00
29.00	3844.00	41.00	4782.00	52.00	79.00	63.05	31.00
30.00	340.00	42.00	2433.00	53.00	770.00	63.95	7.00
31.00	1109.00	43.00	3901.00	54.05	1664.00	65.05	149.00
32.95	5.00	44.00	2945.00	55.05	3979.00	66.05	260.00
33.85	2.00	45.00	1212.00	56.05	917.00	67.10	2113.00
35.05	0.00	46.00	37.00	57.00	9999.00	68.10	5776.00
35.90	2.00	47.00	24.00	58.00	1660.00	69.05	670.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
70.10	1347.00	82.15	418.00	92.20	8.00	103.15	2.00
71.10	4118.00	83.10	245.00	93.10	29.00	104.25	1.00
72.10	765.00	84.10	73.00	94.15	11.00	106.25	0.00
73.10	63.00	85.15	584.00	95.15	351.00	107.15	2.00
73.95	10.00	86.10	633.00	96.15	3865.00	108.25	1.00
75.00	3.00	87.15	35.00	97.15	364.00	109.00	1.00
76.10	2.00	88.10	1.00	98.10	14.00	109.30	0.00
77.10	99.00	89.05	2.00	99.15	106.00	110.00	1.00
78.10	18.00	89.75	1.00	100.05	3.00	110.25	1.00
79.10	328.00	90.00	2.00	101.10	1.00	111.30	3.00
81.15	6242.00	91.10	29.00	102.90	2.00	112.15	31.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
113.15	65.00	128.95	1.00	151.05	1.00	210.45	1.00
114.15	428.00	131.00	3.00	152.40	0.00	219.10	2.00
115.15	32.00	131.80	1.00	153.80	0.00	219.95	0.00
116.15	4.00	133.05	1.00	164.05	0.00	228.95	1.00
117.00	3.00	134.75	1.00	169.05	2.00	234.95	1.00
117.20	1.00	135.65	0.00	169.90	1.00		
118.15	5.00	139.40	1.00	170.40	1.00		
119.05	2.00	144.65	1.00	175.90	1.00		
121.80	0.00	145.05	1.00	181.05	0.00		
122.15	1.00	147.05	1.00	200.45	1.00		
128.65	1.00	149.90	1.00	204.20	0.00		

#146: 2-PENTANONE
Modified: scaled

Entry Number 146 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 18.949
Mol Formula C5H10O
Mol Weight 86.072

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.95	134.00	37.00	36.00	47.95	1.00	59.00	24.00
27.00	1082.00	37.95	74.00	49.00	5.00	59.80	0.00
28.00	129.00	38.95	488.00	50.00	18.00	60.05	2.00
29.00	224.00	39.95	75.00	51.00	13.00	60.95	4.00
29.95	10.00	40.95	1000.00	52.00	4.00	62.05	4.00
31.00	30.00	42.00	455.00	53.00	35.00	62.95	4.00
33.30	0.00	43.00	9999.00	54.05	5.00	63.85	1.00
34.05	1.00	44.00	231.00	55.00	42.00	65.00	5.00
34.25	1.00	45.00	56.00	56.00	5.00	66.05	1.00
34.45	2.00	46.00	1.00	57.05	31.00	67.10	14.00
35.95	3.00	47.60	0.00	57.95	657.00	68.00	3.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
69.00	7.00	78.40	0.00	89.15	0.00	104.75	0.00
71.05	553.00	79.95	0.00	89.45	0.00	105.25	0.00
72.05	26.00	81.05	1.00	91.50	0.00	105.95	0.00
73.05	2.00	81.90	0.00	92.60	0.00	106.60	0.00
74.10	0.00	82.20	1.00	93.40	0.00	107.05	0.00
74.60	0.00	82.95	0.00	97.25	0.00	107.40	0.00
75.05	1.00	83.20	0.00	97.65	0.00	108.00	0.00
75.30	0.00	84.00	1.00	100.65	0.00	108.40	0.00
75.60	0.00	86.10	1016.00	100.90	0.00	108.65	0.00
76.75	0.00	87.10	61.00	102.65	0.00	109.05	0.00
77.00	0.00	88.10	4.00	103.20	0.00	109.50	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
110.20	0.00	121.90	0.00	132.05	0.00	147.15	0.00
112.20	0.00	122.65	0.00	132.90	0.00	147.30	0.00
114.00	0.00	123.10	0.00	133.60	0.00	149.60	0.00
114.55	0.00	123.55	0.00	134.05	0.00	150.05	0.00
115.30	0.00	123.85	0.00	134.90	0.00	152.05	0.00
116.25	0.00	125.15	0.00	137.85	0.00	152.80	0.00
116.85	0.00	127.70	0.00	138.25	0.00	153.40	0.00
117.75	0.00	128.25	0.00	138.50	0.00	154.65	0.00
118.40	0.00	128.40	0.00	142.30	0.00	154.90	0.00
120.10	0.00	129.45	0.00	144.15	0.00	155.15	0.00
121.20	0.00	130.05	0.00	145.05	0.00	155.40	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
155.65	0.00	184.40	0.00	216.05	0.00	248.85	0.00
161.90	0.00	185.80	0.00	219.05	0.00		
162.30	0.00	186.30	0.00	219.90	0.00		
166.10	0.00	188.00	0.00	223.55	0.00		
166.80	0.00	190.90	0.00	224.30	0.00		
170.00	0.00	191.70	0.00	225.80	0.00		
170.60	0.00	197.95	0.00	227.30	0.00		
173.30	0.00	203.55	0.00	234.80	0.00		
175.65	0.00	210.55	0.00	242.20	0.00		
175.85	0.00	211.55	0.00	242.60	0.00		

180.05	0.00	214.10	0.00	248.55	0.00

#147: 3-METHYLCYCLOHEXANONE
Modified: scaled

Entry Number 147 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 44.13
Mol Formula C7H12O
Mol Weight 112.088

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.10	4.00	38.00	207.00	49.95	101.00	61.00	10.00
26.00	233.00	39.00	2608.00	51.00	164.00	62.00	22.00
27.00	2051.00	40.00	692.00	52.00	67.00	63.00	35.00
28.00	692.00	41.00	5540.00	53.00	397.00	64.00	6.00
29.00	1107.00	42.00	4493.00	54.05	190.00	65.05	62.00
30.00	25.00	43.00	1117.00	55.00	4103.00	66.00	33.00
31.00	26.00	44.00	25.00	56.05	4738.00	67.10	419.00
33.05	18.00	44.95	7.00	57.05	410.00	68.10	976.00
34.00	15.00	46.05	1.00	58.00	73.00	69.00	9999.00
35.95	1.00	47.05	3.00	59.05	5.00	70.05	916.00
37.00	68.00	48.95	14.00	60.05	1.00	71.00	74.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
72.05	4.00	83.15	295.00	93.15	18.00	106.90	0.00
73.00	2.00	84.10	416.00	94.15	404.00	107.25	0.00
74.00	6.00	85.10	28.00	95.15	41.00	108.00	1.00
75.00	3.00	86.05	3.00	97.15	896.00	109.20	1.00
75.95	1.00	87.00	1.00	98.15	58.00	110.15	5.00
77.00	30.00	88.25	0.00	99.15	3.00	112.15	2344.00
78.15	31.00	89.00	1.00	102.75	0.00	113.15	196.00
79.15	576.00	89.75	0.00	103.90	0.00	114.10	11.00
80.15	40.00	90.10	1.00	104.25	0.00	115.15	1.00
81.15	47.00	91.15	6.00	105.80	0.00	116.50	0.00
82.15	24.00	92.10	1.00	106.15	0.00	116.90	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
118.95	0.00	133.05	0.00	152.80	0.00	176.40	0.00
121.65	0.00	134.90	0.00	153.15	1.00	181.15	0.00
124.35	0.00	136.30	0.00	154.40	0.00	193.70	0.00
124.90	0.00	137.30	0.00	154.65	0.00	194.95	0.00
126.75	0.00	140.80	0.00	155.05	0.00	196.45	0.00
127.00	0.00	141.15	0.00	164.15	0.00	196.70	0.00
129.00	0.00	147.10	0.00	165.05	0.00	197.05	0.00
129.25	0.00	148.60	0.00	168.30	0.00	197.30	0.00
129.65	0.00	149.30	0.00	170.55	0.00	198.45	0.00

129.90	0.00	150.00	1.00	173.40	0.00	199.55	0.00
131.80	0.00	151.20	0.00	176.05	0.00	201.20	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
207.05	0.00						
212.05	0.00						
213.80	0.00						
217.30	0.00						
220.20	0.00						
223.05	0.00						
225.95	0.00						
226.70	0.00						
238.55	0.00						

#148: DIHYDRO-3-METHYL-2(3H)-FURANONE
Modified: scaled

Entry Number 148 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 50.659
Mol Formula C5H8O2
Mol Weight 100.052
Miscellaneous Information
Aldrich: alpha-methyl-gamma-butyrolactone

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.10	24.00	36.95	142.00	48.00	4.00	59.05	2.00
26.00	850.00	38.00	268.00	48.95	28.00	60.05	3.00
27.00	3023.00	39.00	2267.00	50.00	104.00	60.95	1.00
28.00	2785.00	40.00	906.00	50.95	87.00	61.95	0.00
29.00	1618.00	41.00	9999.00	52.00	33.00	62.55	0.00
29.95	96.00	42.00	3886.00	53.00	209.00	63.15	1.00
31.00	139.00	43.00	1004.00	54.00	116.00	63.90	0.00
33.05	4.00	44.00	86.00	55.05	1213.00	64.75	1.00
33.95	17.00	44.95	60.00	56.10	5562.00	66.00	2.00
35.00	4.00	46.00	2.00	57.10	240.00	67.00	1.00
36.00	15.00	46.95	1.00	58.05	8.00	67.25	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
68.00	9.00	79.40	0.00	93.15	0.00	103.00	1.00
69.00	33.00	81.00	3.00	93.65	0.00	104.45	0.00
70.00	31.00	82.10	1.00	94.50	0.00	104.75	0.00
71.00	167.00	83.10	3.00	94.80	0.00	105.65	0.00
72.10	11.00	84.25	0.00	96.25	0.00	106.40	0.00
72.95	31.00	85.05	2.00	97.00	1.00	110.35	0.00
74.05	2.00	86.05	0.00	98.10	2.00	111.45	0.00
75.05	1.00	87.45	0.00	99.15	73.00	114.65	0.00

77.10	0.00	88.90	0.00	100.10	909.00	115.15	1.00
78.25	0.00	90.65	0.00	101.10	83.00	115.50	0.00
78.40	0.00	90.95	1.00	102.15	7.00	115.95	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
116.40	0.00	134.55	0.00	150.10	0.00	205.20	0.00
116.75	0.00	138.55	0.00	151.15	0.00	206.45	0.00
117.05	0.00	138.80	0.00	153.05	0.00	208.05	0.00
120.15	0.00	141.15	1.00	153.40	0.00	209.30	0.00
124.75	0.00	141.40	0.00	163.90	0.00	214.20	0.00
126.05	0.00	143.80	0.00	165.65	0.00	216.05	0.00
126.50	0.00	144.55	0.00	169.05	0.00	216.95	0.00
128.40	0.00	144.90	0.00	181.65	0.00	222.75	0.00
130.15	0.00	146.15	0.00	181.95	0.00	223.55	0.00
132.80	0.00	146.85	0.00	182.40	0.00	224.95	0.00
134.30	0.00	148.65	0.00	184.55	0.00		

#149: 1-NITROHEXANE
Modified: scaled

Entry Number 149 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 53.009
Mol Formula C6H13NO2
Mol Weight 131.093

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.05	194.00	36.95	22.00	48.00	6.00	59.00	595.00
27.00	2717.00	37.95	71.00	49.00	5.00	60.00	105.00
28.00	728.00	39.00	1477.00	50.00	39.00	61.05	41.00
29.00	3294.00	40.05	276.00	51.00	70.00	62.00	714.00
30.00	667.00	41.00	6016.00	52.00	31.00	63.00	18.00
31.00	490.00	42.10	1086.00	53.00	234.00	64.00	5.00
33.00	15.00	43.00	9999.00	54.10	188.00	65.00	25.00
34.00	1.00	44.00	395.00	55.00	4429.00	66.05	11.00
35.10	0.00	45.00	576.00	56.05	966.00	67.05	154.00
35.35	0.00	46.00	256.00	57.10	1325.00	68.10	117.00
36.05	1.00	46.95	5.00	58.05	114.00	69.05	339.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
70.10	150.00	80.10	5.00	91.00	0.00	101.10	1.00
71.10	40.00	81.15	29.00	91.50	1.00	102.15	45.00
72.05	42.00	82.15	46.00	92.40	0.00	103.10	2.00
73.05	25.00	83.15	187.00	92.90	0.00	104.30	0.00
73.95	12.00	84.10	78.00	93.15	0.00	104.65	0.00
75.00	33.00	85.10	373.00	94.10	2.00	106.15	0.00
76.00	1.00	86.10	46.00	95.10	1.00	106.65	0.00

77.05	7.00	87.15	1.00	96.10	15.00	106.90	0.00
77.95	1.00	88.10	83.00	97.15	2.00	110.65	0.00
78.20	0.00	89.10	12.00	98.10	7.00	112.15	18.00
79.10	13.00	90.15	1.00	99.05	3.00	113.15	2.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
114.15	2.00	130.05	1.00	144.30	0.00	190.70	0.00
115.00	0.00	131.00	0.00	145.15	0.00	207.00	0.00
116.00	0.00	132.10	7.00	147.10	0.00	211.30	0.00
119.00	0.00	132.90	0.00	149.30	0.00	213.45	0.00
120.20	0.00	133.30	1.00	151.05	0.00	217.30	0.00
122.65	0.00	134.05	0.00	154.90	0.00	229.30	0.00
123.50	0.00	139.15	0.00	161.15	0.00	239.45	0.00
125.25	0.00	139.40	0.00	163.90	0.00	243.20	0.00
125.75	0.00	139.80	0.00	173.40	0.00		
128.20	0.00	140.05	0.00	176.05	0.00		
129.25	0.00	142.05	0.00	186.30	0.00		

#150: 5-ETHYL-DIHYDRO-2(3H)-FURANONE
Modified: scaled

Entry Number 150 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 58.84
Mol Formula C6H10O2
Mol Weight 114.067

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.10	8.00	35.00	1.00	46.00	0.00	55.05	1277.00
25.95	549.00	36.00	3.00	46.95	0.00	56.00	2554.00
27.00	2606.00	37.00	48.00	47.35	0.00	57.00	2788.00
28.00	2907.00	38.00	114.00	47.60	0.00	58.00	231.00
29.00	7958.00	39.00	1000.00	48.00	2.00	59.10	235.00
30.00	323.00	40.00	200.00	48.95	9.00	59.95	40.00
31.00	247.00	41.00	1069.00	50.00	49.00	60.95	9.00
32.90	3.00	42.00	2233.00	51.00	57.00	62.00	9.00
33.65	0.00	43.00	297.00	52.05	23.00	62.95	11.00
34.00	4.00	44.00	38.00	53.00	131.00	64.05	2.00
34.75	0.00	45.00	40.00	54.05	80.00	65.00	11.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
66.00	4.00	76.00	0.00	80.05	0.00	90.00	0.00
67.05	44.00	76.10	0.00	81.05	3.00	90.20	0.00
68.05	17.00	76.30	0.00	82.05	2.00	90.65	0.00
69.00	25.00	76.75	0.00	83.00	9.00	91.25	0.00
70.10	1177.00	77.05	0.00	85.00	9999.00	91.65	0.00
71.10	83.00	77.90	0.00	86.10	1035.00	92.20	0.00

72.05	63.00	78.15	0.00	87.10	76.00	93.20	1.00
73.05	11.00	78.75	0.00	88.10	4.00	93.90	0.00
73.95	1.00	79.05	1.00	88.90	0.00	95.10	34.00
75.35	0.00	79.40	0.00	89.15	0.00	96.10	3.00
75.50	0.00	79.75	0.00	89.40	0.00	97.15	14.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
98.05	1.00	110.00	0.00	119.75	0.00	132.40	0.00
98.15	1.00	110.25	0.00	122.00	0.00	134.40	0.00
99.10	3.00	110.90	0.00	122.75	0.00	135.05	0.00
100.05	0.00	111.30	0.00	123.65	0.00	137.40	0.00
100.65	0.00	112.15	2.00	124.75	0.00	138.40	0.00
100.90	0.00	113.15	71.00	125.00	0.00	139.90	0.00
101.45	0.00	114.10	155.00	125.50	0.00	141.35	0.00
105.15	0.00	115.15	39.00	125.90	0.00	144.05	0.00
106.05	0.00	116.15	3.00	126.40	0.00	144.40	0.00
107.05	0.00	117.50	0.00	128.75	0.00	146.55	0.00
108.65	0.00	117.75	0.00	129.00	0.00	146.90	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
147.20	0.00	171.55	0.00	192.80	0.00	215.45	0.00
151.05	0.00	175.80	0.00	200.30	0.00	217.45	0.00
151.30	0.00	179.80	0.00	202.70	0.00	220.00	0.00
151.55	0.00	180.30	0.00	204.55	0.00	221.45	0.00
157.65	0.00	181.80	0.00	204.80	0.00	224.05	0.00
158.70	0.00	182.55	0.00	207.15	0.00	233.30	0.00
160.05	0.00	183.65	0.00	207.55	0.00	243.45	0.00
163.30	0.00	185.25	0.00	207.80	0.00	244.20	0.00
164.10	0.00	185.40	0.00	209.95	0.00		
164.90	0.00	185.55	0.00	210.20	0.00		
169.10	0.00	191.45	0.00	211.30	0.00		

#151: 1-METHYLCYCLOPENTANOL
Modified: scaled

Entry Number 151 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 30.339
Mol Formula C6H12O
Mol Weight 100.088

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.10	12.00	36.95	47.00	47.85	4.00	59.00	453.00
26.00	236.00	38.00	125.00	49.00	16.00	60.00	25.00
27.00	1533.00	39.00	1438.00	50.00	106.00	61.00	9.00
28.00	497.00	40.00	240.00	51.00	160.00	62.00	14.00
29.00	1630.00	41.00	2061.00	52.00	57.00	63.00	25.00

30.10	74.00	42.00	432.00	53.00	369.00	64.05	5.00
31.00	411.00	43.00	9117.00	54.00	128.00	65.00	95.00
33.00	7.00	44.00	276.00	55.00	867.00	66.05	33.00
34.10	3.00	45.00	426.00	56.05	140.00	67.00	1314.00
34.90	1.00	46.00	10.00	57.00	1926.00	68.10	73.00
36.00	3.00	46.95	20.00	58.00	7058.00	69.00	29.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
71.00	9999.00	82.15	99.00	95.00	1.00	110.40	1.00
72.05	710.00	83.15	258.00	96.40	1.00	111.15	1.00
73.00	44.00	85.15	1368.00	97.00	3.00	114.25	1.00
74.00	8.00	86.15	75.00	98.00	1.00	115.00	1.00
74.95	3.00	87.15	6.00	99.15	4.00	117.20	0.00
76.10	1.00	87.80	0.00	100.10	171.00	118.40	1.00
77.15	44.00	88.90	1.00	101.00	13.00	119.00	1.00
78.15	12.00	91.15	1.00	102.15	2.00	121.15	1.00
79.15	88.00	91.90	1.00	102.90	1.00	124.90	1.00
80.00	9.00	93.20	0.00	103.65	0.00	133.15	1.00
81.15	75.00	94.00	1.00	106.90	1.00	134.05	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
135.05	1.00	176.15	1.00				
136.90	1.00	180.15	1.00				
139.90	1.00	185.15	1.00				
142.90	1.00	185.40	1.00				
149.15	1.00	185.95	1.00				
151.05	1.00	194.05	1.00				
154.15	1.00	219.05	1.00				
154.40	1.00						
159.05	1.00						
169.05	0.00						
173.80	1.00						

#152: DIHYDRO-2-METHYL-3(2H)-FURANONE
Modified: scaled

Entry Number 152 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 31.76
Mol Formula C5H8O2
Mol Weight 100.052
Miscellaneous Information
Aldrich: 2-methyltetrahydrofuran-3-one

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	894.00	38.95	184.00	50.00	39.00	60.85	1.00
27.00	2147.00	40.00	43.00	50.95	26.00	61.05	3.00

28.00	4874.00	41.00	185.00	52.00	12.00	62.05	3.00
29.00	3341.00	42.00	852.00	53.00	69.00	62.85	1.00
30.00	105.00	43.00	9999.00	54.00	50.00	63.95	1.00
31.00	339.00	44.00	2211.00	55.00	208.00	64.75	0.00
33.00	2.00	45.00	1916.00	56.00	204.00	65.05	1.00
35.00	27.00	45.95	42.00	57.00	216.00	67.05	1.00
35.85	5.00	47.00	4.00	58.00	147.00	68.00	3.00
37.00	48.00	47.90	2.00	58.95	7.00	69.00	27.00
37.95	65.00	49.00	13.00	60.00	2.00	70.05	12.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
71.10	17.00	82.10	0.00	94.05	0.00	103.90	0.00
72.05	3207.00	83.05	2.00	94.65	0.00	104.15	0.00
73.10	140.00	84.05	2.00	95.20	1.00	105.55	1.00
74.10	9.00	85.05	37.00	96.10	4.00	106.75	0.00
74.85	0.00	86.05	2.00	97.00	0.00	109.65	0.00
76.35	1.00	87.25	1.00	98.05	9.00	110.50	0.00
77.40	0.00	89.15	0.00	100.10	1692.00	111.00	0.00
78.15	0.00	89.90	0.00	101.10	91.00	112.15	0.00
78.40	0.00	91.15	0.00	102.10	8.00	113.00	0.00
79.25	1.00	91.90	1.00	103.15	0.00	113.75	0.00
81.00	1.00	93.00	1.00	103.65	0.00	116.00	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
119.00	1.00	131.00	2.00	150.90	0.00	169.80	0.00
120.50	0.00	131.80	0.00	155.30	0.00	170.15	0.00
121.65	0.00	132.30	0.00	156.80	0.00	174.15	0.00
122.85	0.00	134.90	0.00	163.05	0.00	174.40	0.00
125.00	0.00	137.85	1.00	163.40	0.00	175.40	0.00
125.90	0.00	139.15	0.00	163.65	0.00	178.30	0.00
127.00	0.00	141.05	0.00	164.05	0.00	179.15	0.00
128.65	0.00	141.55	0.00	166.40	0.00	182.75	0.00
129.40	0.00	142.15	0.00	168.30	0.00	183.55	0.00
129.75	0.00	145.80	0.00	168.55	0.00	188.20	0.00
130.00	0.00	147.05	0.00	169.05	0.00	195.20	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
219.05	0.00						
232.95	0.00						

#153: 2-HEPTANONE
Modified: scaled

Entry Number 153 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 37.299
Mol Formula C7H14O
Mol Weight 114.103

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	98.00	38.00	44.00	49.00	2.00	60.00	37.00
27.00	1084.00	39.00	611.00	50.00	22.00	61.00	5.00
28.00	183.00	40.00	98.00	51.00	35.00	62.10	4.00
29.00	975.00	41.00	1046.00	51.95	10.00	63.00	5.00
30.00	32.00	42.10	502.00	53.00	85.00	64.00	1.00
31.00	46.00	43.00	9999.00	54.05	25.00	65.10	8.00
33.00	2.00	44.00	273.00	55.00	357.00	66.00	3.00
34.00	4.00	45.00	62.00	56.05	88.00	67.10	15.00
35.10	1.00	46.00	2.00	57.10	186.00	68.10	5.00
35.85	0.00	47.00	0.00	58.00	5676.00	69.00	13.00
37.00	15.00	48.00	6.00	59.00	1009.00	71.10	1211.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
72.10	353.00	85.10	208.00	97.15	6.00	115.15	50.00
73.10	16.00	86.15	37.00	99.15	187.00	116.15	4.00
74.00	2.00	87.15	2.00	100.10	12.00	117.15	0.00
75.25	0.00	88.00	0.00	101.15	1.00	119.05	1.00
77.00	4.00	88.25	0.00	104.25	0.00	124.40	0.00
78.15	1.00	91.05	0.00	105.25	0.00	128.75	0.00
79.00	5.00	92.40	0.00	105.50	0.00	129.15	0.00
80.15	1.00	93.00	0.00	107.90	0.00	134.55	0.00
81.15	29.00	94.20	0.00	109.90	0.00	136.30	0.00
82.10	3.00	95.15	4.00	112.15	1.00	140.15	0.00
83.00	3.00	96.10	13.00	114.15	264.00	146.80	0.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
148.55	0.00	195.45	0.00				
150.05	0.00	195.80	0.00				
153.15	0.00	213.95	0.00				
153.40	0.00						
155.15	0.00						
157.05	0.00						
157.90	0.00						
163.40	0.00						
167.55	0.00						
181.30	0.00						
190.70	0.00						

#154: 4-METHYLCYCLOHEXANOL
Modified: scaled

Entry Number 154 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 43.859
Mol Formula C7H14O

Mol Weight 114.103

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	164.00	38.10	82.00	49.00	7.00	60.00	10.00
27.00	1806.00	39.00	1602.00	50.00	74.00	61.00	5.00
28.00	579.00	40.00	291.00	51.00	140.00	62.00	11.00
29.00	3221.00	41.00	4069.00	52.00	54.00	63.00	27.00
30.00	240.00	42.00	1194.00	53.00	530.00	64.00	3.00
31.00	745.00	43.00	1469.00	54.00	491.00	65.00	101.00
33.00	5.00	44.00	1617.00	55.00	2737.00	66.10	81.00
33.85	2.00	45.00	306.00	56.10	1054.00	67.00	880.00
35.00	4.00	46.00	14.00	57.00	9999.00	68.10	816.00
35.75	2.00	47.00	14.00	58.00	4388.00	69.05	223.00
36.95	22.00	47.95	7.00	59.00	222.00	70.10	2401.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
71.10	906.00	84.15	41.00	97.15	177.00	109.95	1.00
72.10	48.00	85.15	233.00	98.15	7.00	111.00	2.00
73.10	106.00	86.10	168.00	99.15	11.00	112.15	23.00
74.10	9.00	87.15	8.00	101.50	1.00	113.15	71.00
74.95	4.00	88.00	1.00	102.15	1.00	114.15	30.00
77.00	69.00	89.05	1.00	102.50	1.00	115.15	3.00
78.15	13.00	91.10	25.00	102.90	1.00	115.90	1.00
79.15	247.00	92.15	3.00	106.15	1.00	117.65	1.00
81.15	4639.00	93.15	37.00	107.25	1.00	117.90	1.00
82.15	305.00	95.15	373.00	108.00	1.00	119.05	1.00
83.15	144.00	96.15	1927.00	109.00	1.00	119.75	1.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
120.00	1.00	167.90	1.00				
120.40	1.00	169.10	0.00				
122.95	0.00	176.40	1.00				
129.40	1.00	176.65	1.00				
139.40	1.00	186.20	1.00				
143.15	1.00	186.95	1.00				
143.40	1.00	188.70	1.00				
145.15	1.00	203.05	1.00				
151.10	0.00	207.80	1.00				
151.40	1.00	220.05	1.00				
160.15	1.00	231.80	1.00				

#155: 4-OXO-PENTANOIC ACID
Modified: scaled

Entry Number 155 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 64.329

Mol Formula C5H8O3
Mol Weight 116.046
Miscellaneous Information
Aldrich: levulinic acid

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
25.10	43.00	37.00	28.00	48.00	6.00	59.00	3.00
26.00	333.00	38.00	55.00	48.25	5.00	59.95	49.00
27.00	1027.00	39.00	201.00	49.00	11.00	61.00	126.00
28.00	900.00	40.00	19.00	50.00	31.00	62.10	3.00
29.00	955.00	41.00	163.00	51.00	29.00	63.10	4.00
30.00	70.00	42.00	584.00	52.00	15.00	65.00	6.00
31.00	123.00	43.00	9999.00	53.00	60.00	66.00	3.00
32.00	35.00	44.00	461.00	55.00	813.00	67.00	7.00
33.85	7.00	45.00	960.00	56.00	2877.00	68.10	12.00
34.75	4.00	46.00	33.00	57.00	190.00	69.00	7.00
36.00	13.00	47.00	22.00	58.10	17.00	70.00	54.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
71.10	114.00	81.10	10.00	92.75	2.00	103.00	3.00
72.10	33.00	81.95	10.00	93.40	3.00	103.25	1.00
73.00	491.00	83.10	13.00	94.15	3.00	103.65	2.00
74.10	115.00	84.00	2.00	95.15	5.00	105.15	7.00
75.10	8.00	85.10	3.00	96.15	3.00	108.25	3.00
77.15	6.00	85.95	2.00	97.00	10.00	109.00	3.00
77.95	2.00	87.15	4.00	98.15	76.00	109.30	2.00
79.10	4.00	88.15	5.00	99.10	103.00	111.00	3.00
79.75	2.00	89.00	1.00	100.05	8.00	112.15	4.00
80.15	3.00	90.25	2.00	101.15	145.00	113.90	2.00
80.40	3.00	91.00	5.00	102.15	7.00	115.15	3.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
116.15	148.00	131.80	3.00	156.65	2.00	224.80	2.00
117.00	10.00	134.05	2.00	158.65	2.00	225.05	2.00
118.15	7.00	136.30	2.00	164.40	2.00		
119.00	11.00	139.05	2.00	164.65	2.00		
120.00	2.00	141.30	2.00	165.05	2.00		
120.90	3.00	143.05	3.00	165.30	2.00		
122.15	3.00	146.95	1.00	169.05	5.00		
125.05	0.00	148.80	2.00	181.05	3.00		
126.75	2.00	149.05	2.00	192.70	2.00		
128.25	3.00	150.05	1.00	203.80	2.00		
129.25	4.00	151.15	3.00	213.95	2.00		

#156: 1,2-EPOXYHEXANE
Modified: scaled

Entry Number 156 from C:\DATABASE\hjf.l
CAS 000000-00-0

Melting Point -300
Boiling Point -300
Retention Index 27.149
Mol Formula C6H12O
Mol Weight 100.088
Miscellaneous Information
(hexyl oxirane)

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	383.00	38.00	224.00	50.00	89.00	61.25	4.00
27.00	4510.00	39.00	3131.00	51.00	118.00	62.00	17.00
28.00	1035.00	40.00	666.00	52.00	43.00	63.10	12.00
29.00	6066.00	41.00	8269.00	53.00	519.00	63.95	8.00
29.95	318.00	42.00	9382.00	54.10	238.00	64.95	65.00
30.95	2527.00	43.00	2670.00	55.00	4775.00	66.00	20.00
32.00	12.00	44.00	529.00	56.05	528.00	67.00	513.00
33.00	19.00	45.00	518.00	57.00	1504.00	68.10	279.00
35.50	4.00	46.10	12.00	58.00	4626.00	69.05	290.00
36.10	5.00	47.00	4.00	59.00	272.00	71.05	9999.00
37.00	75.00	49.00	19.00	60.00	14.00	72.10	502.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
73.00	46.00	85.15	501.00	98.05	1.00	112.15	3.00
74.10	6.00	86.15	45.00	99.15	40.00	112.90	2.00
76.00	4.00	88.05	2.00	100.05	10.00	113.40	2.00
77.15	9.00	89.00	2.00	101.00	4.00	114.15	5.00
78.15	2.00	91.25	5.00	104.90	3.00	121.15	2.00
79.00	21.00	92.25	2.00	105.15	2.00	121.50	2.00
80.25	6.00	95.15	3.00	105.50	3.00	125.25	2.00
81.15	45.00	95.50	3.00	106.30	0.00	126.00	2.00
82.15	31.00	95.90	1.00	109.15	2.00	127.65	2.00
83.00	15.00	96.40	2.00	110.15	4.00	131.80	3.00
83.95	26.00	97.00	5.00	111.00	4.00	135.80	2.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
143.40	2.00	176.05	3.00				
143.90	2.00	218.95	4.00				
145.05	2.00						
146.15	0.00						
147.15	3.00						
148.65	2.00						
150.05	4.00						
154.90	2.00						
157.65	2.00						
167.15	2.00						
170.30	3.00						

#157: 1-OCTANOL
Modified: scaled

Entry Number 157 from C:\DATABASE\hjf.l
CAS 000000-00-0
Melting Point -300
Boiling Point -300
Retention Index 52.82
Mol Formula C8H18O
Mol Weight 130.134

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
26.00	170.00	39.00	1633.00	51.00	72.00	62.00	3.00
27.00	2791.00	40.05	375.00	52.00	37.00	63.00	7.00
28.00	672.00	41.00	8711.00	52.95	350.00	63.90	3.00
29.00	4821.00	42.00	5748.00	54.05	486.00	65.00	42.00
30.00	161.00	43.00	7225.00	55.00	7840.00	66.00	25.00
31.00	3062.00	44.00	568.00	56.05	9999.00	67.05	490.00
32.00	60.00	45.00	371.00	57.05	3224.00	68.05	1435.00
33.00	18.00	46.00	18.00	58.10	165.00	69.05	5083.00
35.25	3.00	47.10	3.00	59.00	35.00	70.10	5158.00
36.10	1.00	48.00	5.00	60.10	9.00	71.10	641.00
36.95	13.00	50.00	26.00	60.90	1.00	72.05	42.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
73.10	165.00	84.15	3191.00	95.15	22.00	108.75	2.00
74.00	2.00	85.15	214.00	96.10	7.00	110.25	10.00
75.25	1.00	85.95	6.00	97.15	221.00	111.15	10.00
76.00	1.00	87.15	5.00	98.15	24.00	112.15	72.00
77.15	23.00	88.25	3.00	99.15	4.00	113.15	8.00
78.00	8.00	89.40	2.00	100.10	17.00	114.25	4.00
79.10	37.00	91.00	6.00	101.00	1.00	117.00	2.00
79.95	7.00	92.00	4.00	102.40	2.00	117.25	2.00
81.10	82.00	93.15	6.00	103.65	2.00	125.30	0.00
82.15	699.00	93.40	6.00	107.15	0.00	128.00	2.00
83.15	2660.00	93.90	6.00	108.00	3.00	128.25	2.00
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
129.15	4.00	204.70	2.00				
131.90	2.00	219.05	1.00				
133.15	2.00	224.05	2.00				
135.15	3.00	224.95	2.00				
137.05	2.00						
147.05	3.00						
150.80	2.00						
164.15	2.00						
181.05	2.00						
188.80	2.00						
194.80	3.00						