

LUND UNIVERSITY
FACULTY OF SCIENCE

Furan

A Future Fuel and its Lifetime in Urban Air

**Bachelor Thesis in
Atmospheric Chemistry and Physics**

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Abstract

With a rising global mean temperature caused by increased emission of greenhouse gases into the atmosphere biofuels are considered as a possible solution to the greenhouse effect. One of the potential biofuels is furans and this report aims to determine their lifetime in polluted air. This is done by determining the rate constant of the decay of furan, 2,3-DHF and 2,5-DHF due to reaction with tropospheric ozone. The experiment was performed in a mixture with synthetic air in a 250 L gas cell at 750 ± 10 torr, 298 ± 2 K and scanned by a Fourier Transform Infrared spectrometer. Due to experimental difficulties only two of the three examined rate constants could be determined, these were 2.42 and 4.64×10^{-18} cm³ molecules⁻¹ s⁻¹ for furan and 2,5-DHF, respectively. From these results the atmospheric lifetimes was estimated to be 81 and 4 hours for furan and 2,5-DHF, respectively. Due to their completely different lifetimes furan and DHF are estimated to affect the atmosphere on different scales. Furan is predicted to decay first when it leaves the urban areas and is able to react with OH, while DHF will start to decay as soon as it is emitted and is in contact with ozone. Future work is essential in the understanding of how furans influence the atmospheric chemistry.

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1 Introduction

Since preindustrial time increase human activities have affected the earth's atmosphere more than it is capable of adjusting to. Fossil fuel combustion increases the atmospheric concentration of green house gases (GHG) that causes the global mean temperature to rise. Not only did the industrial revolution mean an increased industrial efficiency, it was also the beginning of modern transportation. The introduction of the relatively cheap fossil fuels allowed a major expansion of the transportation sector, ships and trains soon became the largest emitters of GHG. In the beginning of the 20th century the road transportation grew larger and today it is alone responsible for 75 – 80 % of the transportation sectors emission of carbon dioxide, CO₂ (Uherek et al., 2010).

Since fossil fuels are a limited energy source and its emissions are not a part of the present natural carbon cycle, alternative fuels have been developed the last decades; these are called biofuels. Today there are mainly two different types of biofuels, ethanol and biodiesel (alcohol and ester) on the market. Both of these include an additive in the form of fossil fuel, ethanol contains gasoline and biodiesel a petroleum-based diesel (World watch institute, 2006). Research in this area includes the development of new biofuels but also the understanding of how the existing and upcoming biofuels affect the atmospheric chemistry.

1.1 Background

Ethanol has long been one of the alternatives to gasoline in vehicles and it was not until 2007 that someone questioned the emissions impact on the urban air quality. In the article "Effects of Ethanol (E85) versus Gasoline Vehicles on Cancer and Mortality in the United States" Mark. Z. Jacobson concluded that health risk will become greater with an increased amount of vehicle driven on ethanol in the future. With help from modeled data of how the ethanol use are predicted to increase up to year 2020 Jacobson could estimate future urban ozone levels and the health risk it brings. Ethanol was also found to cause other similar problems by increasing the amount of sulfate and aerosols in urban air.

Today many new biofuels are in the research state, among them are furan, C₄H₄O, a heterocyclic organic compound containing two double bonds, see Figure 1a. By addition of two hydrogen atoms the furan gets more saturated resulting in 2,3- or 2,5-dihydrofuran, C₄H₆O, hereafter referred to as DHF. The difference between the 2,3- and 2,5-DHF is the position of the additional hydrogen atoms, where the numbers indicates on which carbon atoms they are attached to, see Figure 1b and c respectively. The physical and chemical properties of these three furans are presented in Appendix B.1.

Furan is considered both as a biofuel and as an additive to other fuels while 2,3- and 2,5-DHF may be products from different furan combustion. These furans may also be products from other types of furans, such as the completely saturated tetrahydrofuran, C₄H₈, or 2,5 dimethylfuran, see Figure 1e and f respectively.

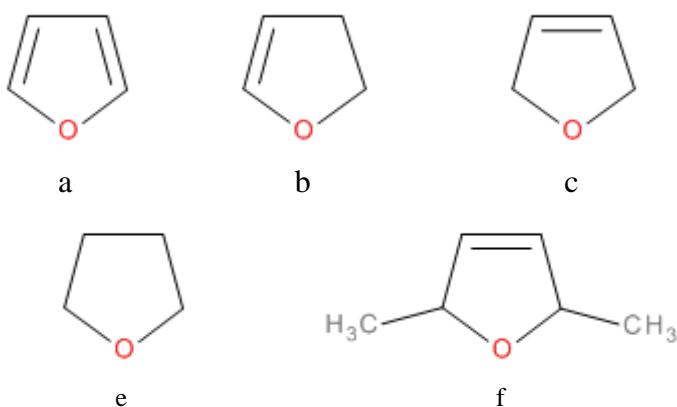


Figure 1 Chemical structure for
a) Furan b) 2,3 DHF c) 2,5 DHF
e) Tetrahydrofuran f) 2,5 Dimethylfuran

Just as for ethanol, new potential biofuels impact on the urban air quality and atmospheric chemistry needs to be examined before put into production. The research needed should include both kinetic and product studies of the biofuels reactions with different atmospheric compounds.

1.2 Previous work

In the early 1980's Adeniji et al. studied the decay of ozone in a polluted atmosphere. In their article "Rate constants for Ozone-Alkene Reactions under Atmospheric Conditions", 1981, they present, among others, the rate constant for the reaction of ozone with 2,5-DHF. Since they were interested in 2,5-DHF's effect on the atmospheric ozone concentration they studied the reaction with 2,5-DHF in abundant. The rate constant is an absolute value and therefore not dependent on the concentration of the compounds; therefore it is the same for the emissions of 2,5- DHF in an ozone rich environment. This rate constant was found to be $16.1 \times 10^{18} \text{ cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$.

In 1983 Atkinson et al. published an article presenting the rate constant for the reaction of furan with ozone. It was found to be $(2.42 \pm 0.28) \times 10^{-18} \text{ cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$. They also studied the reaction of furan with OH and concluded that furan is more reactive towards OH than ozone. In the free atmosphere the OH concentrations are often higher than ozone and furan is therefore more likely to deplete through OH reaction. Atkinson et al. estimated furans atmospheric lifetime to be $\sim 7 \text{ h}$ due to OH reaction, however this may not be the case in polluted urban air where ozone concentrations are high. Atkinson et al. continued their research in the atmospheric reactions between organic compounds and ozone and published in 1984 the article "Kinetics and Mechanisms of the gas-Phase Reactions of Ozone with Organic Compounds under Atmospheric Conditions" that thoroughly examined the mechanism of the reaction between different organic compounds and ozone. Since then furan reaction with ozone have not been examined any further.

1.3 Aim of the study

The aim of this project is to determine the rate constants for the reaction of furan, 2,3- and 2,5-DHF with ozone. With help from these rate constants their lifetimes in urban air can be determined and thereby the local atmospheric impacts of the compounds.

1.4 Disposition

The report begins with two chapters which aim to give the reader a theoretical background of the subject. Chapter 2 gives a brief description of some necessary atmospheric chemistry and chapter 3 describes the chemical kinetics in the project. Chapter 3 also contains a description of the Fourier Transform Infrared spectrometer, FTIR, used to measure the degradation of the investigated compounds. After these two chapters follows a review of the experimental procedure in chapter 4. Finally the results are presented in chapter 5 and discussed in chapter 6.

2 Atmospheric sciences

The atmosphere can be divided into four layers depending on its temperature profile, in atmospheric chemistry the two layers closest to earth are the most important. Due to gravity air pressure are the highest near the ground and falls rapidly with increased altitude. Up to about 10 000 m the temperature falls steady as result of the Ideal gas law.

$$pV = nRT \quad (1)$$

This layer closest to earth is called the troposphere and it is where the weather takes place. In the tropopause, around 10 000 m, the temperature profile becomes relatively constant. Above the tropopause, in the layer called the stratosphere, the temperature starts to rise with increased altitude again. This is due to the absorption of energetic solar radiation during the stratospheric ozone production. Even though the temperature starts to increase above the tropopause, it is sufficiently cold for freeze drying to take place and therefore water rarely manages to reach the stratosphere. Due to the big difference in humidity between the troposphere and the stratosphere their chemistry differs significantly (Seinfeld & Pandis, 2006).

2.1 Hydrocarbon chemistry

Hydrocarbons have a great impact on atmospheric chemistry, both in urban air and on a global scale (Seinfeld & Pandis, 2006). These molecules come from both anthropogenic emissions and are naturally released from vegetation in the biosphere. Most of these hydrocarbons reach the atmosphere in vapor phase and are called Volatile Organic Compounds, VOC.

The hydrocarbons are divided into different classes depending on their functional groups. These determine the molecular physical and chemical properties. The functional groups treated in this report are described in Table 1 below.

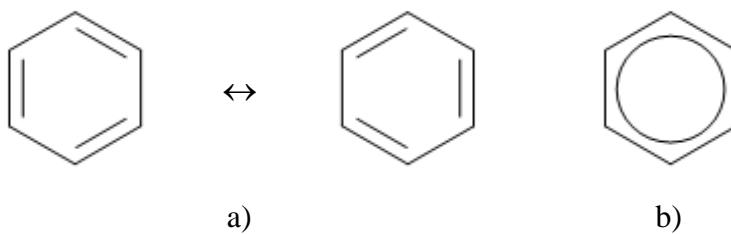
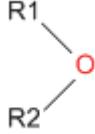
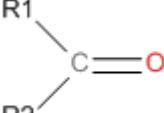
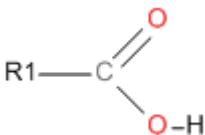


Figure 2. a) The double bonds in a benzene ring b) and its delocalized electrons.

In a molecule the atoms share electrons due to their covalent bindings. A double bond is stronger than the single bond, and a triple bond is even stronger than the double bond. In a cyclic molecule as benzene, see Figure 2, the double bonds result in even stronger attraction than the regular double bond. The explanation is that the electrons are dislocated in the molecule and are therefore not associated with a specific atom creating a stronger bond. The molecules that exhibit these properties are called aromatic organic compounds. Furan can also be seen as aromatic, but is not as stable as benzene.

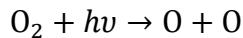
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Table 1. Functional groups examined during the project.

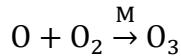
Functional group	Characteristic name
	Ether
	Alcohol
	Ketone (Carbonyl)
	Carboxylic

2.2 Stratospheric ozone

At altitudes around 30 km the incoming solar radiation includes wavelength < 242 nm. This radiation is energetic enough to photolyse oxygen and initiates the Chapman cycle:



In the presence of other atmospheric molecules, M, the free oxygen atom manages to react with oxygen and produce stratospheric ozone:



Depending on the wavelength of incoming radiation the ozone will later on degrade to oxygen and a free or excited oxygen atom:



The excited oxygen atom will eventually collide with surrounding air molecules, loose some of its energy and therefore quench back to its ground state (Seinfeld & Pandis, 2006).

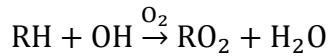
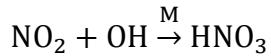
These high stratospheric ozone concentrations are called the ozone layer and it is what is protecting all biological life from the most energetic part of the solar spectrum.

2.3 Tropospheric ozone

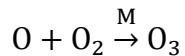
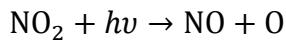
One of the differences between the stratospheric and tropospheric ozone is how it is being produced. In the troposphere ozone is produced as a result of the VOC/NO_x mechanism.

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NO_x , a group name for NO and NO_2 , is released to the atmosphere through the process of combustion. Both NO_x and VOC are highly reactive towards the hydroxyl radical, OH , and there is a constant competition between these two compounds in the troposphere (Seinfeld & Pandis, 2006).



where RH represents the VOC. At high tropospheric VOC concentrations NO_2 does not completely decay through reaction with OH. At wavelength < 424 nm the residual NO_2 is photolysed resulting in a free oxygen atom. In the same manner as in the stratosphere this oxygen atom can collide with oxygen and create an ozone molecule:



Hence, increased emissions of organic compounds can result in severe air pollution.

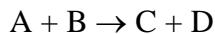
3 Theory

This chapter will give a brief description of the chemistry and physics needed in this project. It is divided into two parts; the first part describes the chemistry behind the reactions, how to estimate their rate constant, the ozone addition to the furans and how to scavenge unwanted products during the experiment. The furan reactions are studied with a Fourier Transform Infrared spectrometer, FTIR. The physics behind this measuring technique is described in the second part of this chapter.

3.1 Chemical kinetics

3.1.1 Second order reaction

This project treats the second-order reaction of furans with ozone. A second-order reaction (bimolecular) means that two compounds react with each other and create two new different compounds (Seinfeld & Pandis, 2006):



The rate of this bimolecular reaction is:

$$\frac{d[A]}{dt} = -k_{2nd} \cdot [A] \cdot [B] \quad (2)$$

When the rate constant for the reaction is determined the lifetime of A, due to reaction with B, can be estimated by:

$$\tau_A = \frac{1}{k_{2nd}[B]} \quad (3)$$

3.1.2 The absolute rate method

With one of the compound concentrations in abundance, and therefore considered constant during the reaction, the absolute rate method can be used for calculating the rate constant. According to (2) the rate for the reaction of [A] with [B] can be described as:

$$\frac{d[A]}{dt} = -k'_{2nd} \cdot [A]$$

where k'_{2nd} contains both the constant [B] and the rate constant k . By solving the inhomogeneous differential equation a linear expression can be concluded.

$$\begin{aligned} [A]_t &= [A]_0 \cdot e^{-k'_{2nd} \cdot t} \\ \ln\left(\frac{[A]_t}{[A]_0}\right) &= -k'_{2nd} \cdot t \end{aligned} \quad (4)$$

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This linear expression is then used when plotting A's degradation as a function of time. The rate coefficient corresponds to the slope of the linear regression that results when all k'_{2nd} are plotted as a function of B's varied concentration. It is important that the investigated reaction is the only reaction that takes place during the experiment, otherwise the absolute rate method is not a valid approximation.

3.2 Furan reaction with ozone

When ozone reacts with a molecule containing a double bond it will attach to that bond as described in Figure 3. Therefore the reaction rate for these types of molecules depends on the properties of the double bond, for example on what atoms it is connected to. This information comes in hand for further product studies of these types of reactions (Atkinson & Carter, 1984)

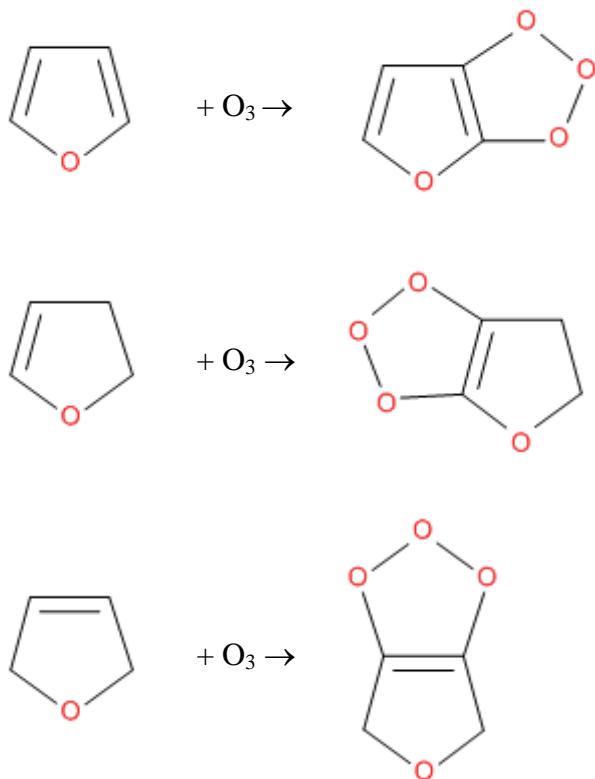


Figure 3. Ozone adding to the double bond in
a) furan b) 2,3 DHF c) 2,5 DHF.

3.2 Cyclohexane reaction with OH

One of the estimated products of the reaction of furan with ozone is the hydroxyl radical, OH, which is also a *probable* reactant with furan in the atmosphere. It is therefore of interest to remove this molecule from the experiment to ensure that this reaction does not take place and influence the desired result. This is done by adding a molecule that is highly reactive towards OH, which therefore never has the possibility to react with another molecule, such as the investigated compounds (Grosjean & Grosjean, 1995).

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In this project that molecule was cyclohexane producing cyclohexanon during the reaction with OH, see R4. The associated mechanism to R4 is presented in Figure 4 below.

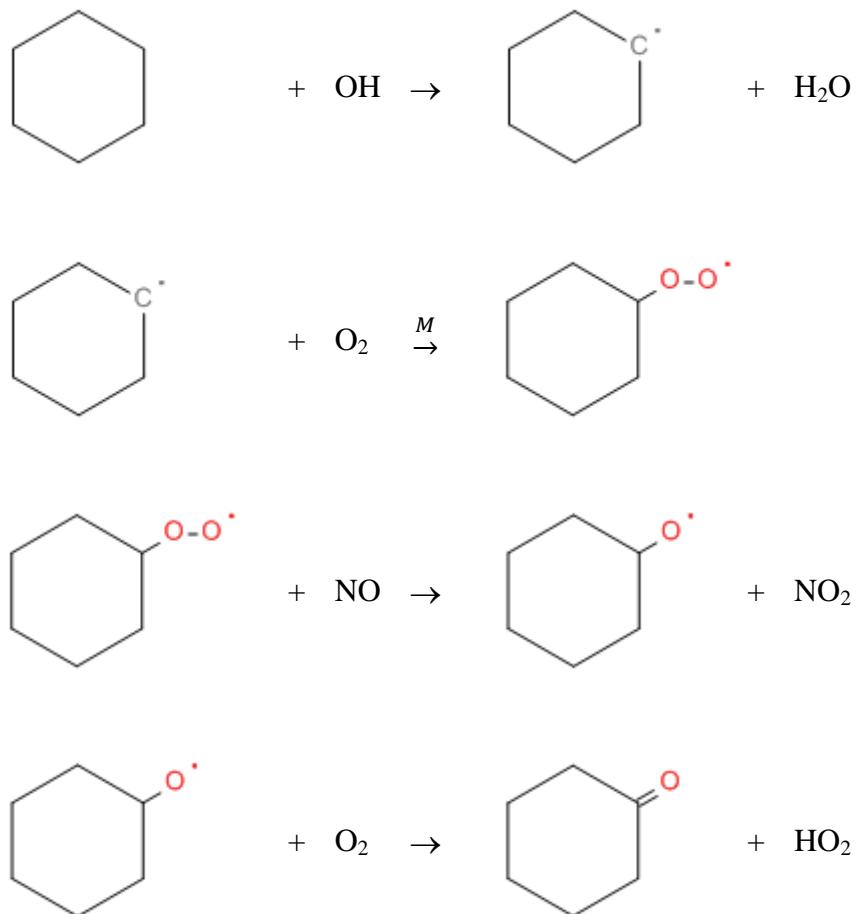


Figure 4. The mechanism of the reaction for cyclohexane with OH.

3.3 Infrared spectroscopy

According to quantum mechanics energy can only be absorbed by a molecule in discrete quanta. When the molecule deexcites it will radiate in the same frequency range as the absorbed energy. These energy spectra are called the molecular absorption spectra. Every molecule has a unique absorption spectrum depending on its rotational mode and vibration of the functional groups and bonds. By studying this spectra information about the molecular structure can be concluded.

Not only the bonds and functional groups affect the absorption spectra; these functional groups can access different vibrational modes making the spectra even more complex, see Figure 5. In organic chemistry most of the molecules have vibrational modes corresponding to the infrared, IR, wavelength region, $4000 - 625 \text{ cm}^{-1}$, hence IR-spectroscopy is suitable for studies of these compounds (Williams & Flemming, 1995).

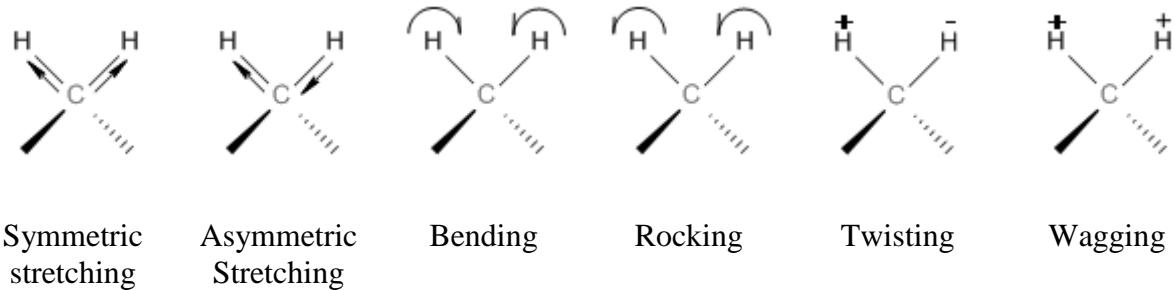


Figure 5. The different localized vibrations a molecule can posses.

A molecule's absorption spectrum mainly contains two regions of information. The region above 1500 cm^{-1} usually consist of information about molecular functional groups and the region below 1500 cm^{-1} is unique for every molecule; it is therefore referred to as the fingerprint region. Once a molecule's fingerprint region is known it can be used as a reference in the analysis of many different experiments.

3.3.1 The Beer-Lambert law

The transmitted intensity of a beam passing through a gas sample is defined as:

$$T = \frac{I}{I_0} \quad (5)$$

where T is called the transmittance, I_0 is the intensity of the incoming light and I is the intensity of the light that has passed through the sample. The transmittance depends on the number of molecules it interacts with along the way. In other words, the transmitted light is proportional to the concentration of the compound in the sample and the optical path length. This is described by the Beer-Lambert law (Atkins & de Paula, 2002):

$$I = I_0 \cdot 10^{-\varepsilon[C]l} \quad (6)$$

where ε is the molar absorption coefficient, $[C]$ is the compound concentration and l is the optical path length. Since the absorbance of that same beam can be described as:

$$A = -\log T = \log \frac{I_0}{I}$$

the Beer-Lambert law can be rewritten as:

$$A = \varepsilon[C]l \quad (7)$$

When simulating atmospheric conditions with low pressure, and therefore low compound concentrations, the path length needs to be long for a sufficiently high absorption to be measured.

Since the absorbance is described as the logarithm of the transmission it can never be larger than 1 in theory. However in practice a lot of samples often reach an absorbance of as much

as 5 in some spectral ranges. This is an instrumental problem that indicates that the absorbance is saturated for that spectral line.

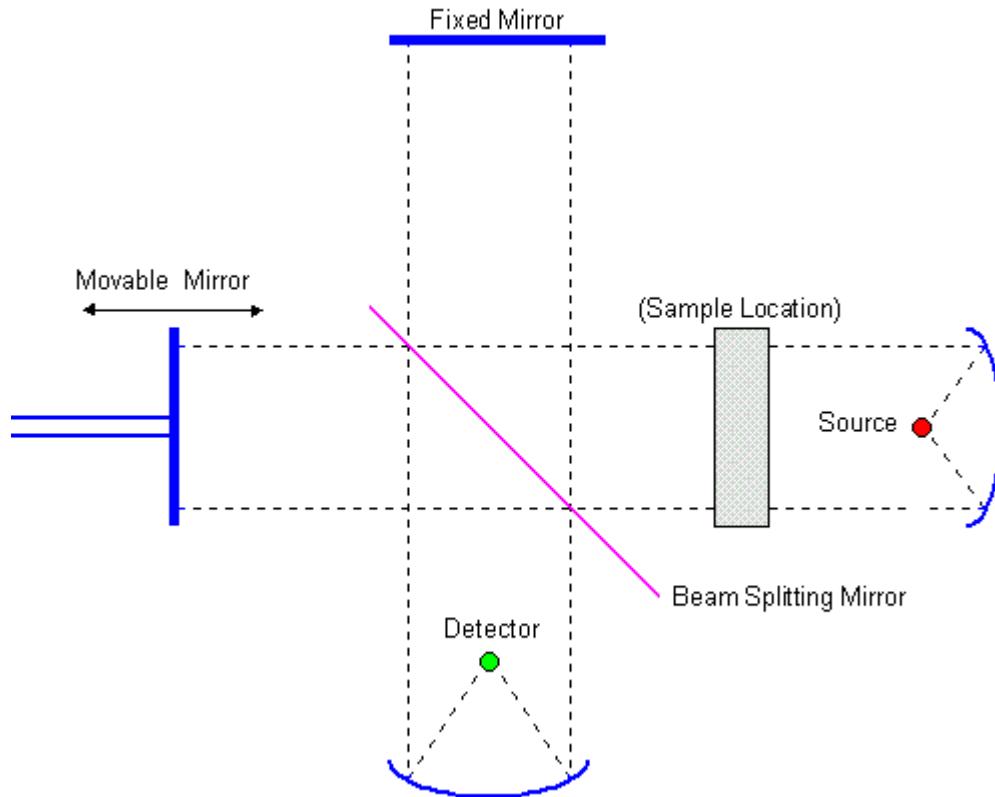


Figure 6. The Fourier Transform Infrared spectrometer. (The picture has been modified
Source: <http://jpkc.henu.edu.cn/sybpfx/scha/images/ir-05.gif>, 2013-06-01)

3.3.2 FTIR

To be able to analyze a wide spectral range at the same time a Michelson interferometer is used. In a FTIR the source emits infrared radiation, and after the beam passed through the sample it is divided by a beam splitter into two perpendicular parts. Each of these is reflected back to the beam splitter and then registered by the same detector, see Figure 6. Since one of the beams hits a movable mirror its path length will vary with the distance of the mirror. When the two beams are recombined they create an interference pattern depending on the different wavelengths that the beam consists of. When the mirror is being moved during a sample period the interference pattern changes and creates a signal called an interferogram. To be able to interpret this signal it needs to be fourier transformed, hence the name FTIR.

3.3.2 Resolution

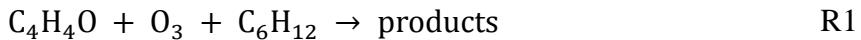
The resolution for a FTIR depends on the difference in optical path length that causes the interferogram according to (Atkins & de Paula, 2002):

$$\Delta\sigma = \frac{1}{2L}$$

where σ is the wave number, measured in cm^{-1} and L is the maximum optical path length. This means that by moving the mirror at least 5 cm one can obtain a resolution of 0.1 cm^{-1} between the absorption bands in the spectra. In addition to the instrumental limits, the spectra contains properties that affect the resolution. The spectral bands can be broadened by Doppler and lifetime broadening. The Doppler broadening is a result of the Doppler effect. The frequencies of the beams can be shifted due to different velocities and moving directions of the molecules in the gaseous sample. Hence Doppler broadening depends on the velocity of the measured molecule and if it is moving towards or away from the detector. The total Doppler broadening is the sum of the Doppler effect for all the molecules. This effect can be reduced by lowering the temperature of the sample resulting in lower velocities. Despite low temperatures the spectral lines can never be infinitely sharp due to the Heisenberg uncertainty principle; this is called the lifetime broadening of a spectral line.

4 Method

The aim of the project is to examine the reactions of furan, 2,3- and 2,5-DHF with ozone, therefore the following reactions were performed in the laboratory:



As described above one of the estimated products is hydroxyl radical. Since OH is also expected to be reactive towards the furans the experiments will include C_6H_{12} , a molecule that scavenge any potential OH.

4.1 Experimental setup

The experiments were performed at the department of Chemistry, University of Oslo. In the same manner as D'Anna et al. performed their experiments in 2008 the measurement took place in a 250 L electropolished stainless steel reactor containing a White-type multiple reflection mirror system resulting in 120 m optical path length. Here the compounds are mixed with synthetic air (20 % O_2 , 80 % N_2) at 750 ± 10 torr, 298 ± 2 K, and then analyzed with an on-line Fourier transform infrared (FTIR) detection. The infrared spectrum is recorded by a Bruker IFS 66, with a resolution that is set to be 0.5 cm^{-1} . (The time of detection is then short enough to obtain a spectrum before the reactants manage to fully react with each other.)

4.2 Experimental procedure

The compounds were connected to the gas cell via a gas handling manifold. Both the manifold and the gas cell were connected to a vacuum pump resulting in extremely low pressure inside the closed system. This lets gas flow from higher pressure through the manifold to the lower pressure inside of the gas cell. The order for the compounds to be injected into the gas cell was as follows; ozone, cyclohexane and finally one of the furans and then fill up with air.

Ozone was produced through discharge in an ozone generator from Ozomax Inc. Pure oxygen was led through the ozone generator which was then connected to a glass tube filled with a silica gel. The glass tube was placed in a solution of dry ice and methanol or propanol resulting in temperatures low enough for the ozone to condensate and attach to the silica gel when flowing through the glass tube. For practical reasons the gas tube was connected directly to the gas cell, hence, the ozone concentrations were never known before the first scan, which only gave a clue of the actual concentration. The concentrations were then adjusted by removing different amounts of ozone from the cell and refilling it with synthetic air.

The gas handling manifold contained a sphere of 0.5 liters that could be isolated from the rest of the system. By filling this reference volume to a certain pressure, the initial concentration of the compound was known before it was swept into the gas cylinder with a low flow of synthetic air. This flow of synthetic air was necessary since the gas cell already contained ozone of a pressure higher than the one inside the manifold. Once inside the cell the compound passed through a perforated pipe to be evenly distributed in the sample. After cyclohexane was placed in the gas cell it was filled with synthetic air to a pressure of 600 – 700 torr. Filling the gas cell to a high pressure before the furans was injected ensured the data sampling to start as close to the initiation of the reaction as possible.

The spectra were scanned 128 times as a standard, which took ~80 s to register. To analyze the decay of the compounds the data sampling were repeated 20 times during a 30 second interval. For some of the faster reactions analyzes were shortened to 30 scans, still repeated 20 times but with a 10 s interval instead. The spectra were then studied in *OPUS*.

Before starting the experiments a first concentration combination for the reaction compounds was estimated to 2 ppm of one of the furans, 20 ppm cyclohexane and 200 ppm ozone. The first reaction to be studied was the reaction of furan with ozone. It was then found that the ozone concentration was far too high since none of the furan in the experiment could be found in the spectra. The ozone concentrations were gradually decreased during the following experiments and the amount of the furans and cyclohexane in the reference volume was set to be 1 and 10 torr respectively as a standard. When it came to the 2,3 and 2,5 DHF the same ozone concentration problem appeared again, but this time with the concentration that had been suitable for furan. The ozone concentrations were then again decreased. The 2,5 DHF started to appear in the spectra, but not the 2,3 DHF. At one time the ozone concentration was so low that the reaction with 2,3 DHF stopped due to ozone deficit.

4.3 Reference spectra

Reference spectra for the analysis were produced in the same gas cell as the experiments took place. Before the experiments, absorption spectra of the compounds were unknown. Therefore an initial concentration was estimated which later on could be varied to fit the spectra. After looking at the reference first spectra it could be decided how to adjust the concentration of the compound; lowering the concentration was easily done by removing a small amount of gas in the cell and the refill it with more synthetic air. Since the absorbance of the compounds varies over the spectral range many reference spectra with different concentrations were recorded to fit the different areas of interest.

During this phase of reference production a spectral area where all the compounds resulted in distinct peaks was found and chosen to be used as an analysis area. $560\text{--}940\text{ cm}^{-1}$ is where the furan, 2,3- and 2,5-DHF peaks are the sharpest and ozone have the lowest absorption. Therefore the references were adjusted to fit this area in particular, see Figure 7-9 below.

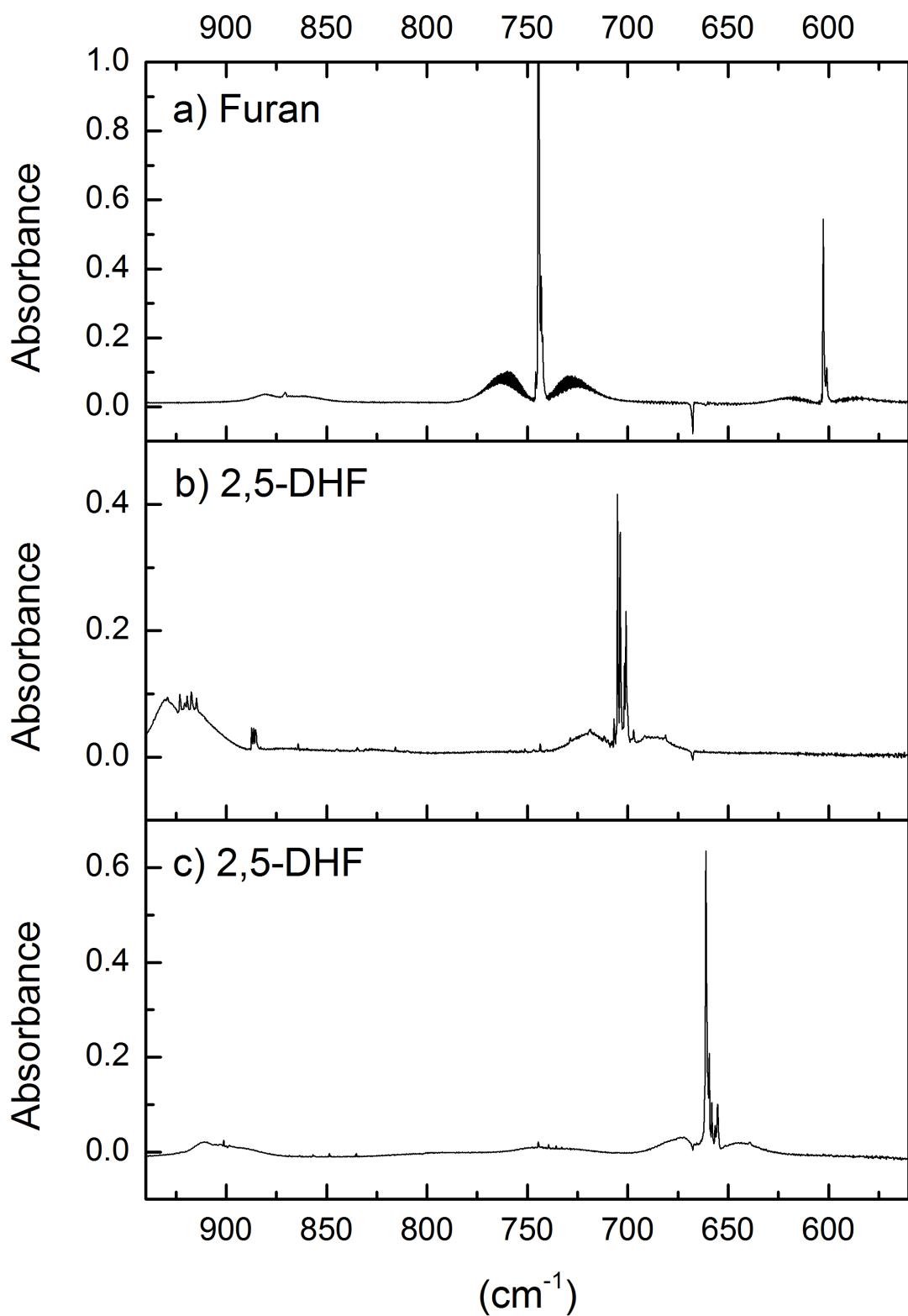


Figure 7. Reference spectra for
a) Furan b) 2,3-DHF c) 2,5-DHF.

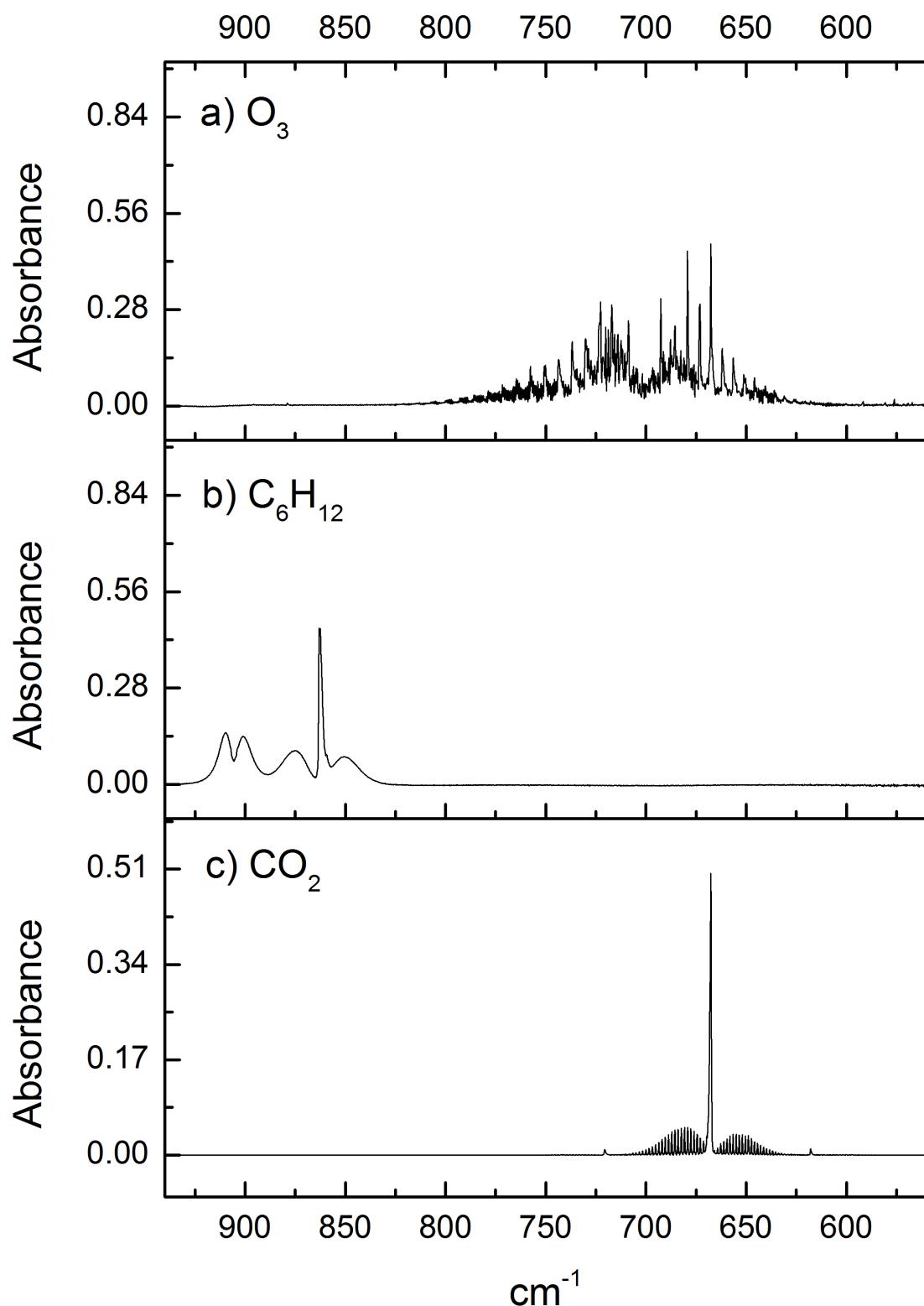


Figure 8. Reference spectra for
a) Ozone b) C₆H₁₂ c) CO₂ (Hitran).

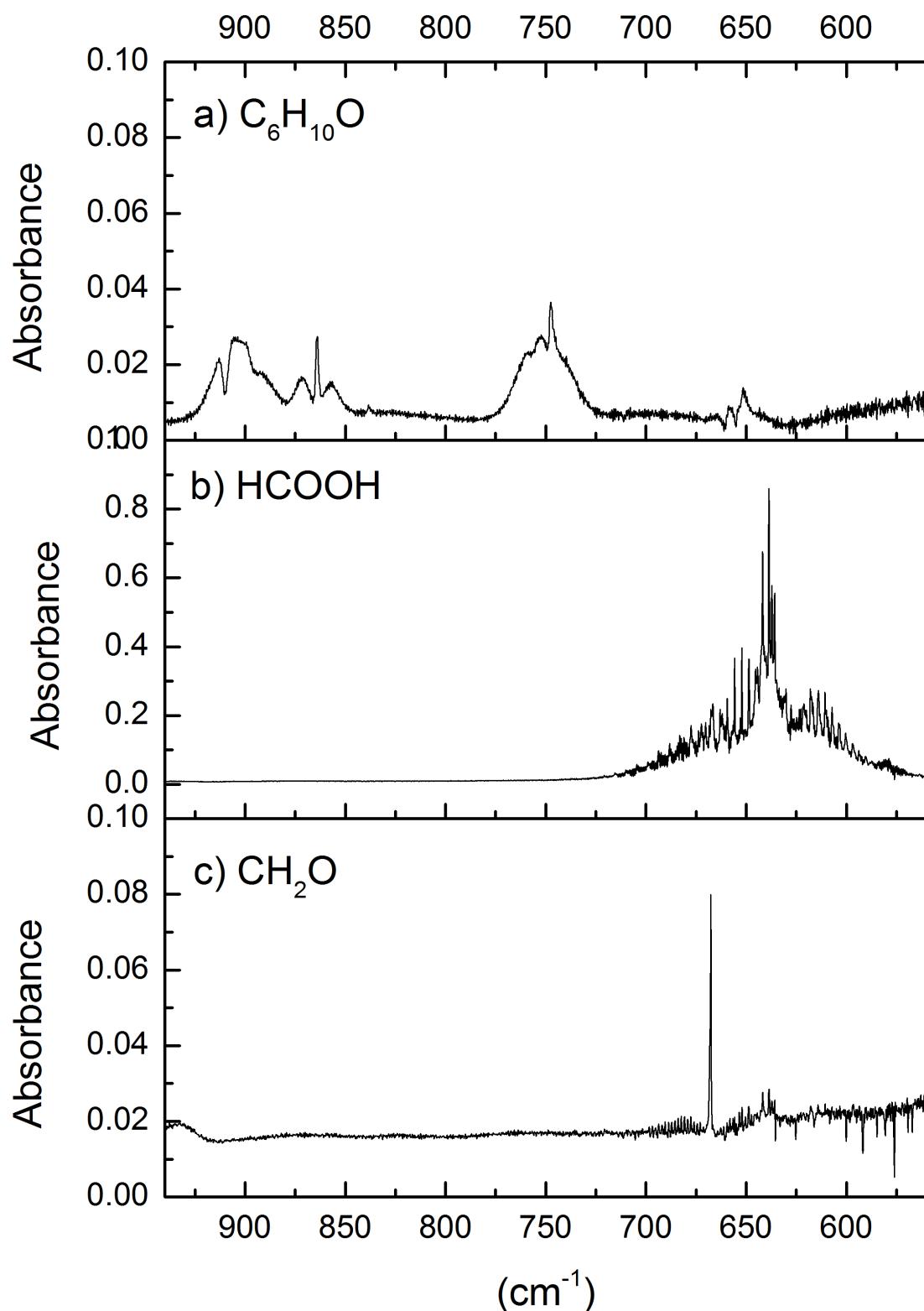


Figure 9. Reference spectra for
a) $\text{C}_6\text{H}_{10}\text{O}$ b) HCOOH c) CH_2O .

4.4 Analysis

The analytical part was performed in *Malt5*, a program that with help from reference spectra of different molecules tries to fit a spectrum to the measured one. In a code, read by *Malt5*, a first estimation of the compound concentrations is made, by adding “true” or “false” *Malt5* is allowed to fit more exact concentrations (Griffith, 1996). *Malt5* also takes instrumental parameters into account; these can also be fitted if necessary. All parameters used in the project are presented in Table 2 below.

The results are three spectra, the measured one, the fitted one and a residual that is the difference between the two first spectra. If the analysis missed a molecule in the fitted spectra this molecule will end up in the residual. Figure 10 illustrates two results from *Malt5*; in the first one CO₂ is not part of the references list. It is quite clear from the residual in the first figure that *Malt5* is not able to identify one of the molecules of the sample during the analysis. In the second one the CO₂ is included as a reference and therefore removed from the residual, but it is still not perfect. The two additional peaks, besides the noise, in the residual is an effect emerging from a small shift between the measured and fitted spectra.

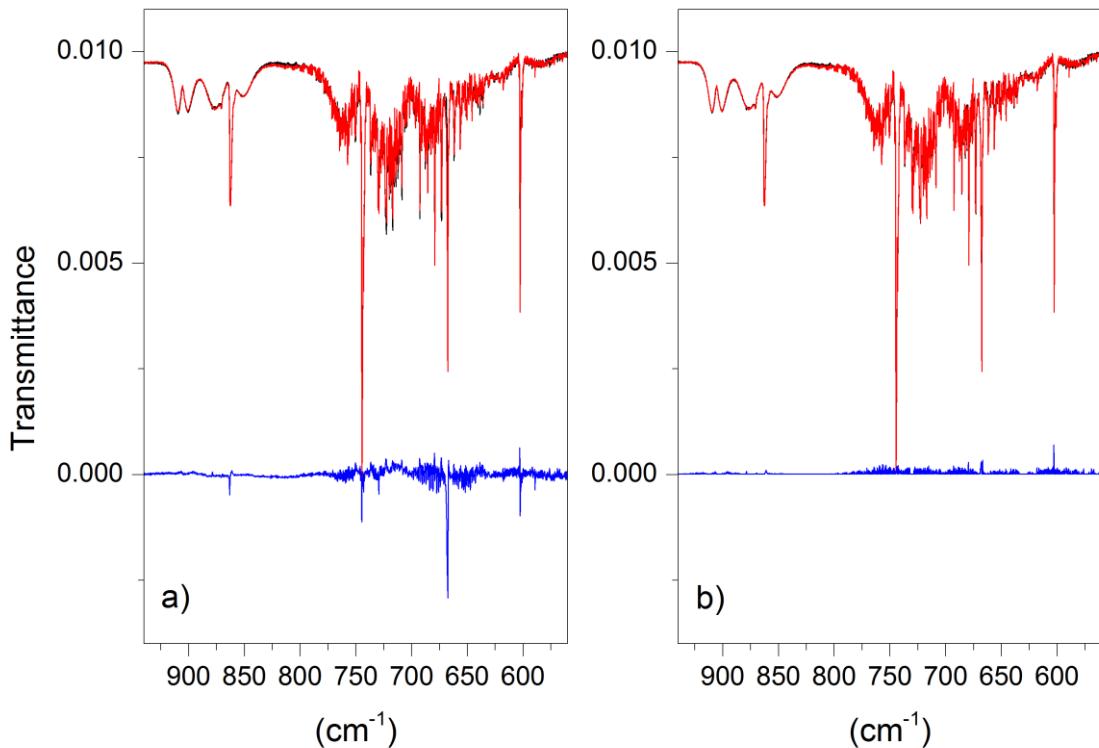


Figure 10. Example of an analytical result from *Malt5*.

- a) Peaks in the residual, the blue spectrum, indicates that the *Malt5* missed a molecule during analysis.
- b) By adding CO₂ to the analysis most of the peaks are removed from the residual.

Reference CO₂ spectra were taken from the Hitran-catalog (High resolution transmission). Since Hitran consists of only the 42 most commonly used molecules the reference list for the analysis needed to be complemented with spectra belonging to the molecules of interest (Rothman, 2009).

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The analyzed spectra were evaluated in *OPUS* before the final result could be plotted in a program called *OriginPro*. In this program mainly three different plots were produced:

1. The varying ozone concentration versus time.
2. The compound degradation versus time.
3. The second order decay versus the varying ozone concentration.

Table 2. The parameters used during analysis in *Malt5*.

<i>Malt5</i> Parameter		Unit	Fitting
Iterations	20		
Intervall	560 – 940	cm ⁻¹	
Path	120	m	
Pressure	750	torr	false
Temperature	298	K	false
<hr/>			
Hitran components			
CO ₂	1	ppm	true
<hr/>			
Reference spectra			
Furan	5	ppm	true
2,3-DHF	5	ppm	true
2,5-DHF	5	ppm	true
O ₃	50	ppm	true
C ₆ H ₁₂	20	ppm	true
HCOOH	2	ppm	true
<hr/>			
Instrument properties			
Shift	0.08	cm ⁻¹	true
Resolution	0.5	cm ⁻¹	false
Field of view	27	cm ⁻¹	false

5.4.1 Conversion of concentration

Malt5 presents all the estimated concentrations in parts per million, which is often used as the standard unit in atmospheric science. But when calculating the rate constants it is more convenient to use SI units. Below follows a derivation on how to convert the results from ppm to SI units.

According to the Ideal gas law (1) the atmospheric number concentration per cubic centimeter can be calculated by:

$$n_{air} = \frac{p_0 N_A}{RT}$$

Constants and properties of the atmosphere and gas cell are presented in table 3.

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Table 3. Properties of the Atmosphere and in the gas cell during the experiments (Seinfeld & Pandis).

Standard atmospheric pressure	p_0	1.01325×10^5	Pa
		760	torr
Pressure in the gas cell	p	750	torr
		1.00×10^5	Pa
Standard atmospheric temperature	T_0	288	K
Temperature in the lab	T	298	K
Avogadro's number	N_A	8.314	J mol ⁻¹ K ⁻¹
Molar gas constant	R	6.022×10^{23}	molecules mol ⁻¹

$$n_{air}(0) = \frac{(1.01325 \times 105 \text{ Pa})(288 \text{ K})}{(8.314 \text{ J mol}^{-1} \text{ K}^{-1})(6.022 \times 10^{23} \text{ molecules mol}^{-1})}$$

$$n_{air}(0) = 2.55 \times 10^{19} \text{ molec cm}^{-3}$$

$$n_{air}(\text{lab}) = \frac{(1.00 \times 105 \text{ Pa})(298 \text{ K})}{(8.314 \text{ J mol}^{-1} \text{ K}^{-1})(6.022 \times 10^{23} \text{ molecules mol}^{-1})}$$

$$n_{air}(\text{lab}) = 2.43 \times 10^{19} \text{ molecules cm}^{-3}$$

The analytical ozone concentrations in ppm are converted to molecules/cm by multiplication with the factor $n_{air}(\text{lab})$ before the rate constant are determined.

5 Results

Two weeks of laboratory measurements resulted in 22 experiments distributed by

- 10 furan reactions with ozone
- 5 2,3-DHF reactions with ozone
- 7 2,5-DHF reactions with ozone

that were suitable for analysis in *Malt5*. From these experiments only 15 made it through the analysis with reasonable resulting compound concentrations. The results are summarized in Table 4 below and corresponding plots are found in Appendix A. Finally the estimated rate constants are presented in Table 5 together with earlier experimental data.

5.1 Furan degradation

During the experimental part of the project, analysis of the spectra started by studying the spectra as they were produced. Reactions that ended before the sample time was over were stopped in advance and samples without any reactions at all were canceled. In this way the sample conditions could be modified for a better result.

Figure 11 is an example of how the spectra looked like during the experiments. In Figure 11a the entire analysis area is studied. With help from the reference spectra, found in section 4.3 above, both the initial compounds and products can be identified. The reaction started with furan, ozone and cyclohexane, which are all marked in the Figure. The remaining peak represents CO₂, who results in a distinct absorption band over this interval according to its reference spectrum.

In this interval furan contains two peaks, one of them saturated in the beginning of the experiment, hence the absorption is far above 1. According to Figure 11b this saturated furan peak more than halved after just one scan, corresponding to 30 seconds. After 60 seconds the peak is down at an absorption around 1 and after 11 scans, about half the sample time, this furan peak is almost eliminated. At the same time as furan is decaying CO₂ is being produced around 668 cm⁻¹, see Figure 11c, and after 90 seconds CO₂ reached saturation.

During the experiment the spectra of cyclohexane remain quite stable, indicating absence of OH production. Even though these spectra look stable at a first sight there is a small fluctuation. At a closer look some of cyclohexanes peaks appear to decay while others stay the same. This may be a result of products being formed, while spectra overlapping with the spectra of cyclohexane.

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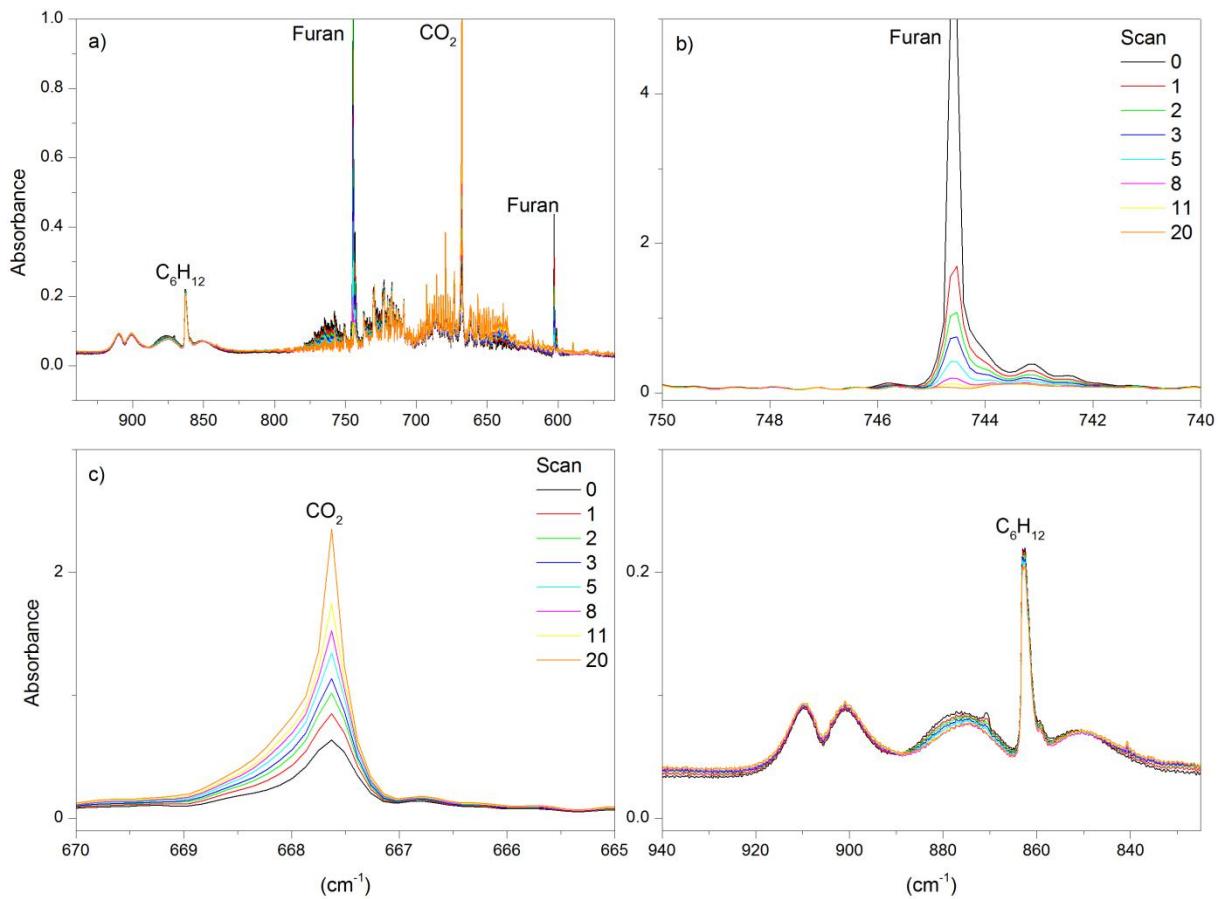


Figure 11. Spectra showing the furan degradation through reaction with ozone during the fourth experiment, 2013-04-26. The Figures presents the spectrum of the scan at the start of the reaction followed by scan nr 1, 2, 3, 5, 8, 11 and 20.

a) Overview of the reaction of furan with ozone in the analyzed area between 940 – 560 cm⁻¹. b) The degradation of the furan peak around 745 cm⁻¹. c) The production of CO₂ peak around 668 cm⁻¹. d) The C₆H₁₂ spectra remain relative stable during the reaction indicating no or relatively small consumption of the compound.

Figure 12a is a good example of one of the difficulties that occurred during the experiment: the first ozone concentrations did not have time to stabilize before the furan reaction was initiated. After the third scan the ozone concentration stabilized around 79 ppm and stayed within the error margins throughout the experiment. This is why the two first scans are left out in the linear regression of the furan decay in Figure 12b. In the end of the experiment the decay rate ceases to be linear indicating additional furan reaction with some of the possible products.

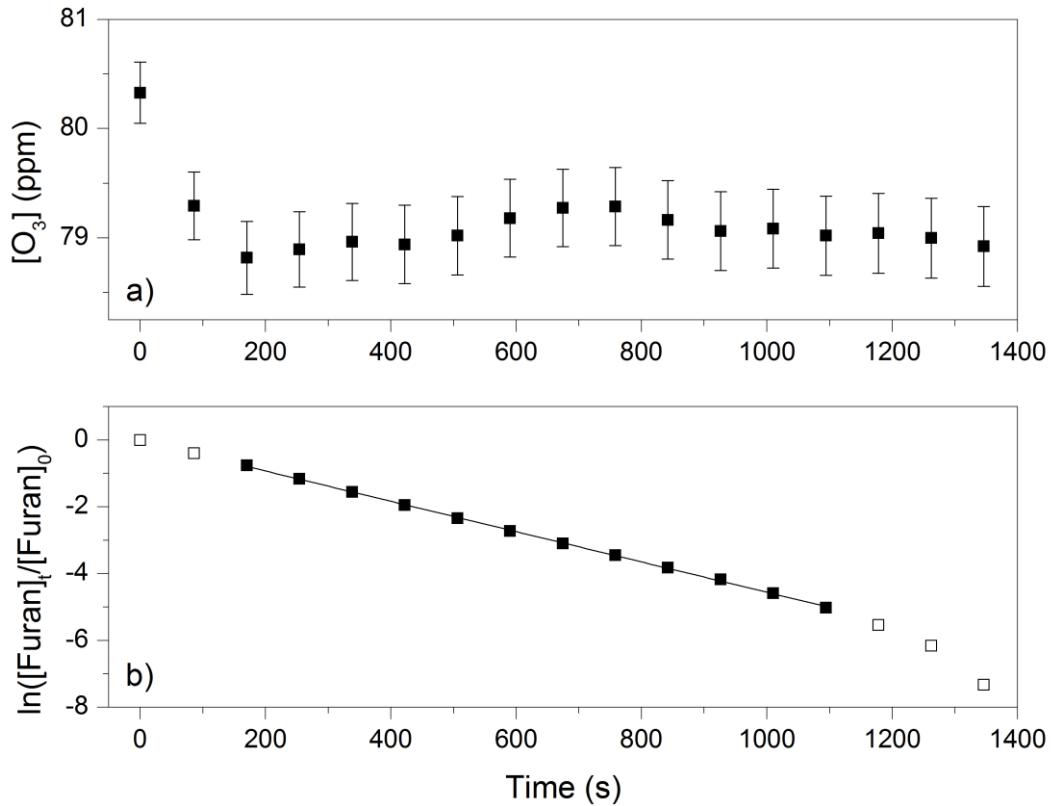


Figure 12. Fourth experiment, 2013-04-26.

- a) Ozone concentration verses time.
- b) Furan decay through ozone reaction versus time.

Similar plots as Figure 12 for the other experiments are found in appendix A. These plots have been used to evaluate which points to use for the decay plots. The constant ozone concentration to be used in the absolute rate method (4) is determined by the mean value of the ozone concentration that does not differ significantly from the rest.

5.2 Rate constants

Table 4. Initial analyzed ozone concentrations and resulting decay of furan, 2,3- and 2,5-DHF. The RMS is a measure of how good the analyzed approximation is estimated to be; a good RMS value is usually < 1 . The result are sorted by date and corresponding experiment order of that day.

Date Experiment	[O ₃] (ppm)	RMS	Slope (10^{-3} s ⁻¹)
Furan			
2013-04-16			
2 nd	99.1 ± 1.5	2.34	- 62.1 ± 0.06
3 rd	47.9 ± 1.5	2.74	- 3.18 ± 0.01
2013-04-18			
3 rd	33.1 ± 0.75	1.62	- 2.96 ± 0.02
4 th	16.3 ± 1.75	1.58	- 1.87 ± 0.00
2013-04-25			
4 th	~ 4.3 ± 0.75	0.88	- 0.21 ± 0.00
5 th	48.1 ± 0.75	0.81	- 3.03 ± 0.06
2013-04-26			
3 rd	54.4 ± 0.5	0.88	- 4.09 ± 0.05
4 th	79.1 ± 0.5	1.08	- 4.54 ± 0.03
5 th	26.1 ± 1	1.08	- 1.02 ± 0.01
2,3 DHF			
2013-04-18			
2 nd	194.6 ± 1	0.89	- 1.44 ± 0.11
2013-04-25			
2 nd	1.0 ± 0.6	1.26	- 1.07 ± 9.35
2,5 DHF			
2013-04-22			
7 th	4.0 ± 0.5	0.98	- 2.54 ± 0.08
2013-04-24			
1 st	2.4 ± 0.5	0.73	- 3.95 ± 0.16
2 nd	12.9 ± 0.3	0.73	- 14.57 ± 0.30
3 rd	5.0 ± 1	0.77	- 5.00 ± 0.03

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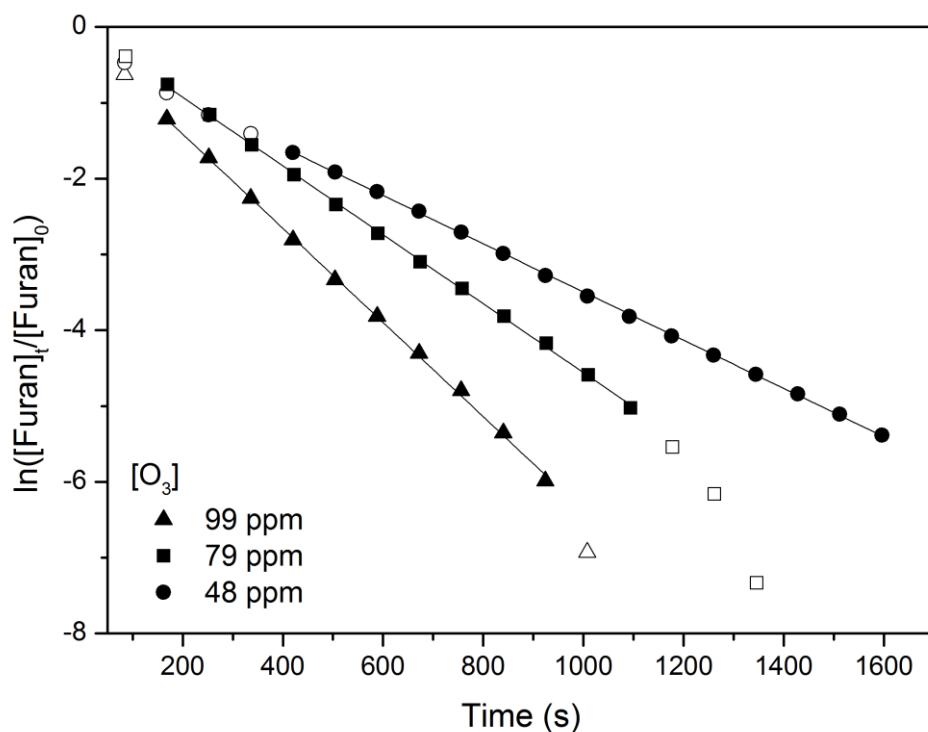


Figure 13. Furan decay through reaction with different concentration of O_3 measured in ppm.

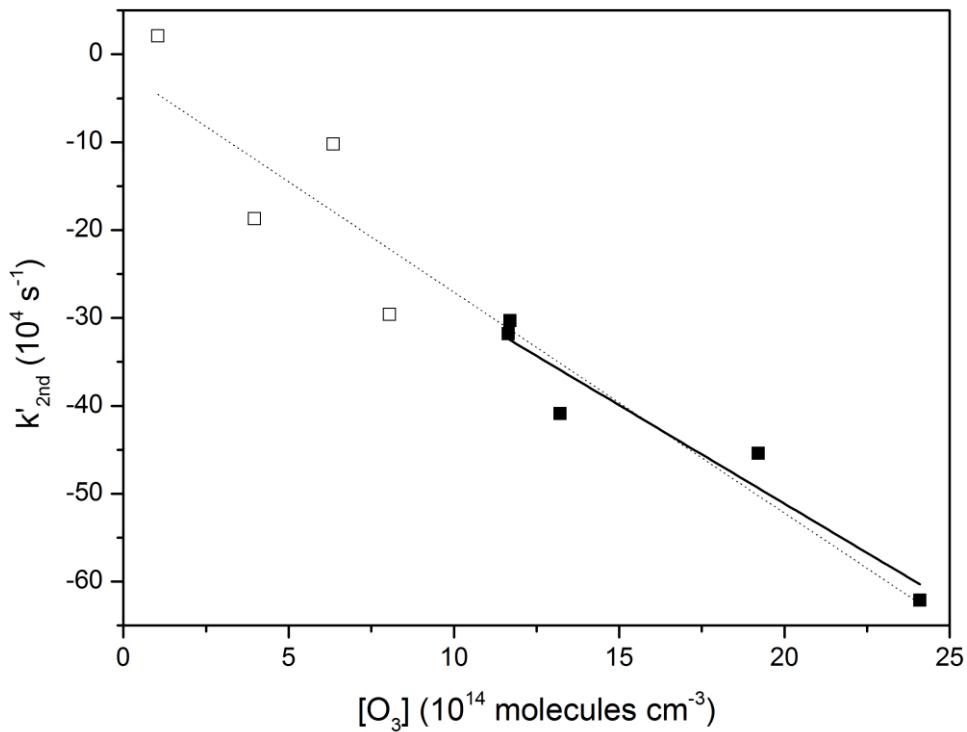


Figure 14. Second-order decay of Furan versus ozone concentration measured in molecules cm^{-3} .

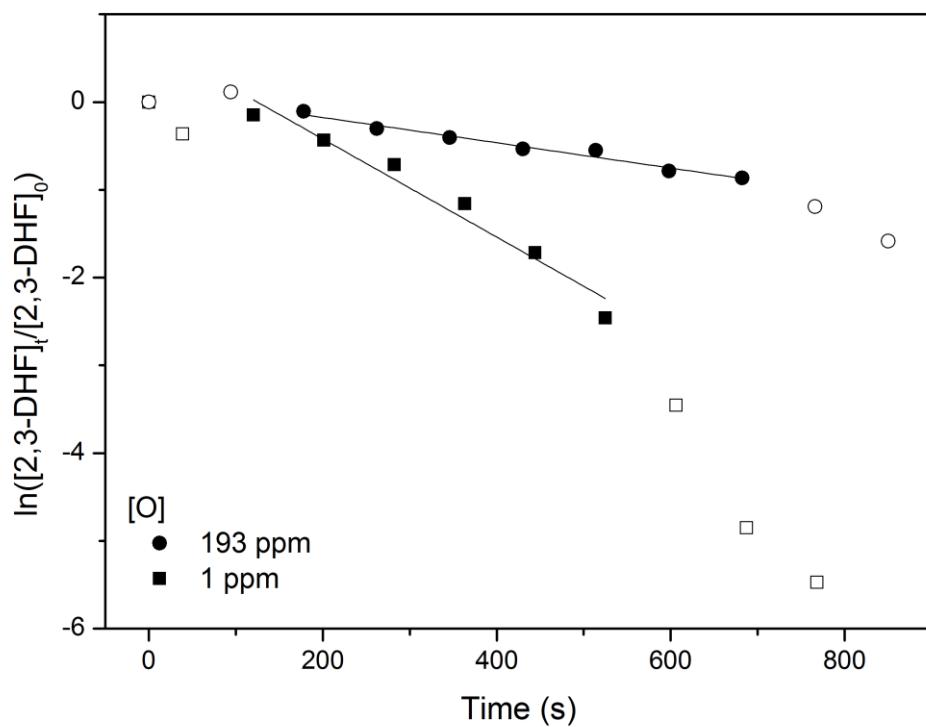


Figure 15. 2,3-DHF decay through reaction with different concentration of O₃ measured in ppm.

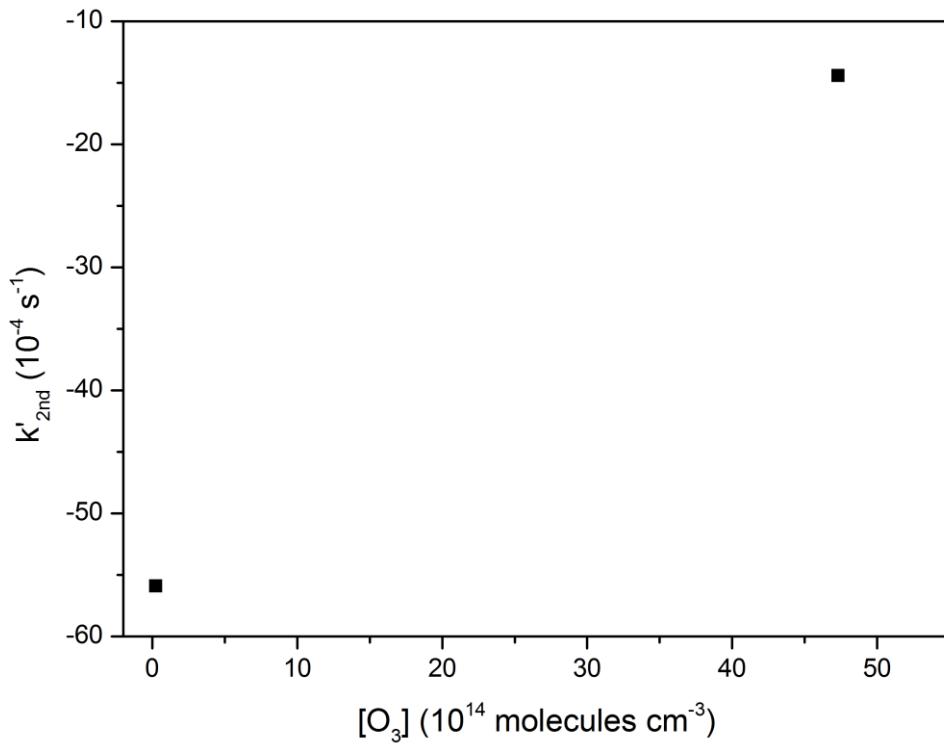


Figure 16. Second-order decay of 2,3-DHF versus ozone concentration measured in molecules cm⁻¹.

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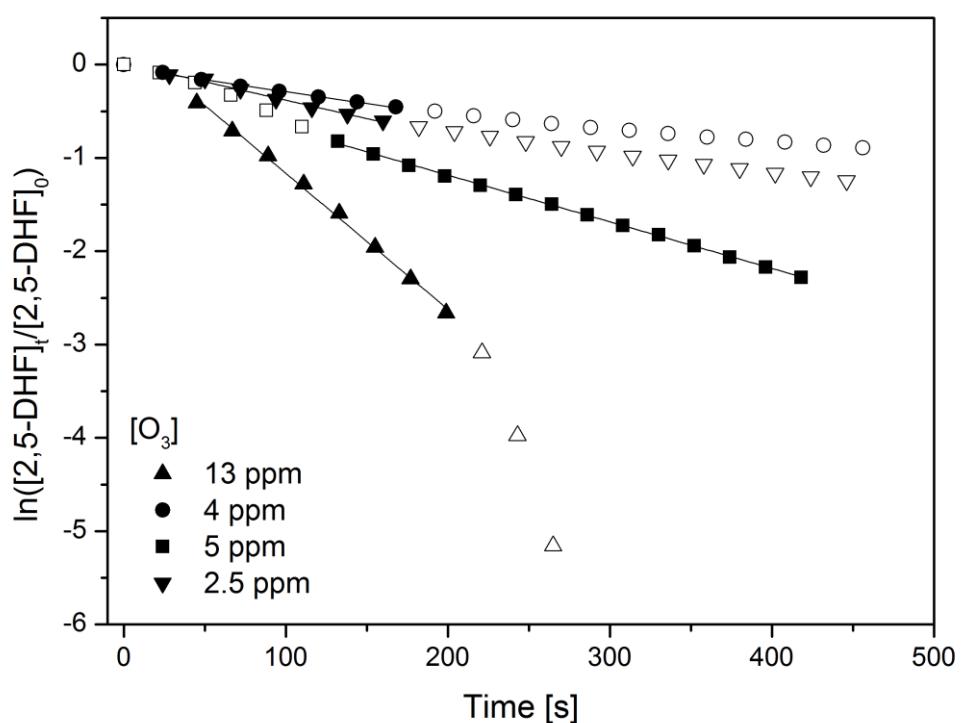


Figure 17. 2,5-DHF decay through reaction with different concentration of O_3 measured in ppm.

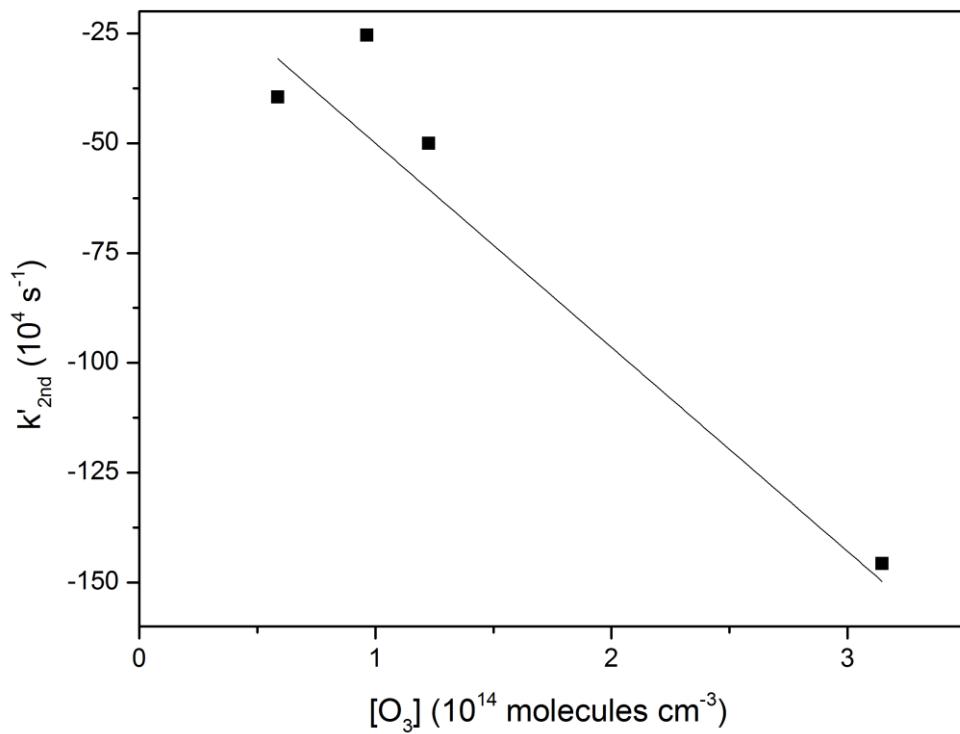


Figure 18. Second-order decay of 2,5-DHF versus ozone concentration measured in molecules cm^{-3} .

Figure 13 presents three of the furan experiments. These three resulted in both relatively stable high enough ozone concentrations and a linear furan decay. For the absolute rate method (4) to be a valid approximation the reactant needs to be in abundance relative to the compound of interest. Since the furan concentration was ~ 5 ppm the ozone concentration limit was set to > 40 ppm being considered abundant.

Two different rate constants are estimated for the reaction of furan with ozone. The dashed line in Figure 14 is the linear regression of the furan decay in all the experiments in Table 4. The solid line represents the three reactions in Figure 13 for the same reasons as described above. The slopes of these lines represent the rate constant for the reaction of furan with ozone and are presented in Table 5. The rate constant for the reactions in Figure 13 was estimated to be $2.42 \times 10^{-18} \text{ cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$. The less reliable rate constant for all the furan reactions was estimated to be $2.51 \times 10^{-18} \text{ cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$ placed inside a parenthesis in Table 5.

As to the reaction of 2,3-DHF with ozone in most of the experiments, ozone concentrations were far too high for this reaction. As a result the decay of 2,3-DHF was never detected since the compound was consumed before the start of the sampling time. Despite this rapid reaction, two of the experiment resulted in concentrations suitable for analysis. The decay of 2,3-DHF is plotted against time in Figure 15 and its linear regression is plotted against the ozone concentration in Figure 16. Since there are only two experiments that came through the analysis it is not possible to calculate a reliable rate constant for the reaction of 2,3-DHF with ozone.

During the experimental phase of the project the spectra for the reaction of 2,5-DHF with ozone indicated the same problem as for 2,3-DHF. But unlike 2,3-DHF the analysis of 2,5-DHF resulted in compound concentrations high enough to estimate a rate constant for the reaction with ozone. Figure 17 presents the decay of 2,5-DHF and include all four experiments in Table 4. With ozone concentrations ranging between 2.5 and 13 ppm none of these experiments consist of ozone in abundance, > 40 ppm. Despite this a rate constant is estimated with the absolute rate method (4) represented by the slope of the linear regression in Figure 18.

The Swedish Meteorological and Hydrological Institute defines an ozone episode as days with an 8 hour average tropospheric ozone concentrations > 60 ppb. When calculation the atmospheric lifetime, according to (3), of furan and 2,5-DHF this threshold value is used for the ozone concentrations. The lifetimes of the compounds was found to be 81 and 4 hours for furan and 2,5-DHF respectively.

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Table 5. Estimated rate constants and resulting atmospheric lifetimes of furan, 2,3- and 2,5-DHF. The atmospheric lifetimes are calculated for ozone levels of 60 ppb. The previous rate constants are retrieved from Atkinson et al. (1983) and Adeniji et al. (1981).

	Furan	2,3-DHF	2,5-DHF
Rate constant [10^{-18} cm 3 molecules $^{-1}$ s $^{-1}$]	2.24 ± 0.37 (2.51) ± (0.30)		46.4 ± 14.5
T (K)	298 ± 2		298 ± 2
p (torr)	750 ± 10		750 ± 10
Lifetime (h)	81		4
<hr/>			
Previous work			
Rate constant [10^{-18} cm 3 molecules $^{-1}$ s $^{-1}$]	2.42 0.28		16.1
T (K)	298 ± 2		294 ± 2
p (torr)	735		760

6 Discussion

Biofuels are today thought to be one possible solution to the global warming. A couple of years ago it was discovered that the most commonly used biofuel today, ethanol, can come to cause severe air pollution in the future. With this fact in mind, the atmospheric chemistry of new biofuels needs to be examined before they are put into production. One of these potential biofuels is furans and this project aimed to determine the rate constants for the reactions of three different furans with ozone. Of the three examined rate constants only two could be determined.

The rate constant for the reaction of furan with ozone resulted within the margin of errors of the previously determined rate constant, see Table 5. This rate constant was estimated in two ways, one by including the furan decay in all experiments. The other included only the experiments that resulted in both relatively stable, and high enough, ozone concentrations and a linear furan decay. Despite this fact, the difference between these two rate constants is very small; within the margin of errors of each other, they can be considered the same.

The estimated rate constant for the reaction of 2,5-DHF with ozone was in the same order of magnitude as previous work, but was about three times faster than previous data. Since the ozone was set at such low concentrations during these experiments, ozone cannot really be considered in abundance compared to 2,5-DHF. This may affect the result since the absolute rate method is only a valid approximation if one of the reactants concentration stay constant throughout the experiment. This was not the case for the ozone concentrations in the 2,5-DHF experiments. Another error for this rate constant is that the decay rates in Figure 18 are not evenly distributed along the linear regression. Three of the experiments are found in an area of the same ozone concentration and the fourth is at the other end of the line. Due to this, the linear regression can be viewed as a result of only two points instead; reducing the credibility of the rate constant for the reaction of 2,5-DHF with ozone. With this information in hand the estimated rate constant for the reaction of 2,5-DHF with ozone in this project should be viewed as an indication of what the proper rate constant is rather then an actual result.

The rate constant for the reaction of 2,3-DHF was never estimated since Figure 16 includes only two decay rates of 2,3-DHF. Taking a closer look at the experimental result in Figure 15 and 16 two additional errors arises:

- 1) The decay plot belonging to the ozone concentration of 1 ppm does not appear to be linear, even though this was the most linear part in the decay plot, see Appendix A.2.
- 2) If an ozone concentration > 100 ppm never was suitable for the other experiments how come that an ozone concentration of 198 ppm came through the analysis with reasonable compound concentrations?

The first observation indicates that 2,3-DHF is reacting with some of the possible products, which makes that experiment unsuitable for the absolute rate method. The second observation is probably a result of an analysis problem which means that the experiment cannot be considered reliable and should be discarded.

At the beginning of the project ozone was thought to be more reactive towards furan than 2,3- and 2,5-DHF. The idea arises from the fact that furan contains two double bonds while 2,3- and 2,5-DHF contains only one double bond each. From this point of view ozone has twice as many opportunities to attack furan and a reaction of ozone with furan should therefore be faster than those with DHF. Since furan is aromatic the atoms are bond stronger in furan than those in DHF and it is therefore easier for ozone to break the double bond in DHF. This can be an explanation as to why ozone reacts faster with 2,3- and 2,5-DHF than with furan.

With a lifetime of 4 hours in a polluted atmosphere 2,5-DHF is never able to leave urban areas. Hence, its reaction with ozone results in local impacts only. Furan on the other hand has a lifetime of 81 hours due to reaction with ozone. With this relatively long lifetime the compound is able to leave the urban areas and affect the atmosphere at a regional scale. Well out in the free atmosphere furan may decay through collision with OH. According to Atkinson et al. this reaction is faster than the ozone reaction, which means that once furan left the polluted area it will soon degrade through reaction with OH. So even if the furan is able to impact the atmosphere at a regional scale it is unlikely for it to result in greater effects on a global scale.

For future studies of these compounds the ozone concentration needs to be made even lower. This means that it will not be possible to calculate the rate constants from the absolute rate method. This can be solved by looking at the ozone reactions with furan, 2,3- or 2,5-DHF in abundance instead. Another way is to use other methods when calculation the rate constants. If the ozone concentrations are to be lowered then the experimental setup may need some modifications so that the ozone concentrations are known before injected into the sample. The unknown ozone concentrations were a major source of error during this project since it complicated the process of testing different ozone concentrations.

Even though the furan experiments resulted in a reliable rate constant it may be complemented with additional experiments with stable ozone concentrations and linear decay as the three experiments in Figure 13. This may strengthen the credibility of the rate constant for the reaction of furan with ozone. As mentioned above the rate constant for the reaction of 2,5-DHF with ozone should be viewed as an indication of what the proper value is. It is therefore recommended that all the 2,5-DHF experiments will be repeated under other conditions. The same applies to the 2,3-DHF reactions as it is of interest to know the difference between the two DHF's rate constants in order to get an proper idea of the chemical properties of the two compounds.

It is also of interest to implement these experiments on other types of furans. With a complete product study of different furans, conclusions can be drawn on how these compounds relate to each other. With help from these product studies the furans impact on the urban air quality can be determined. These product studies can together with information about the compounds atmospheric lifetime estimate the furans influence on the atmospheric chemistry.

7 Conclusions

In a time when a rising global mean temperature threatens the world, research on new biofuels is important. One potential candidate for biofuel is furans. This report aimed to determine the rate constants for the reaction of furan, 2,3- and 2,5-DHF with ozone and thereafter estimate these furans lifetime in polluted air.

The rate constants, due to reaction with ozone, was found to be $2.24 \times 10^{-18} \text{ cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$ and $46.4 \times 10^{-18} \text{ cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$ for furan and 2,5-DHF, respectively. With help from these the lifetime of these compounds was estimated to be 81 and 4 hours for furan and 2,5-DHF, respectively. Due to experimental difficulties the rate constant and its resulting lifetime of 2,3-DHF could never be determined.

The results indicate that furan, due to its aromatic characteristics, is more stable than DHF in the atmosphere. Furan is predicted to decay first when it leaves the urban areas and is able to react with OH, while DHF will start to decay as soon as it is emitted into the atmosphere and come in contact with ozone. Furan will therefore be able to influence the atmospheric chemistry on a larger scale than DHF. At the same time this means that the DHF is more likely to affect the local air quality in urban areas. Future work, such as product studies, is essential for a complete understanding of how furans affect the atmospheric chemistry.

Acknowledgment

The author would like to thank Elna Heimdal Nilson, Lund University, for her support and feedback throughout this project and Claus J. Nielsen, University of Oslo, for the guidance and support during the laboratory experiment in the end of April, 2013.

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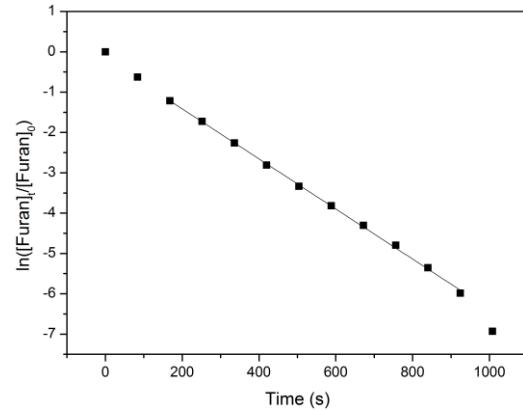
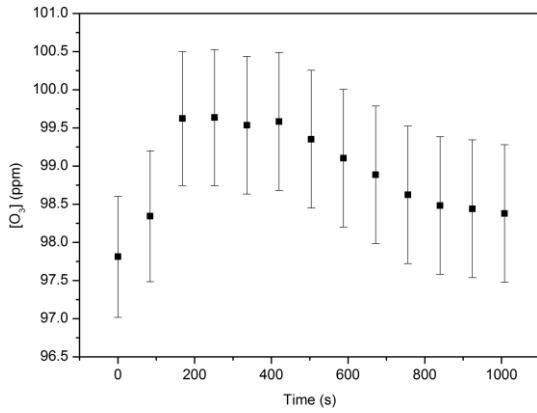
Appendix A

This appendix contains analytical ozone concentrations and compound degradation from each of the experiments. They are categorized in furan, 2,3- and 2,5-DHF, and subcategorized after date and order of experiments.

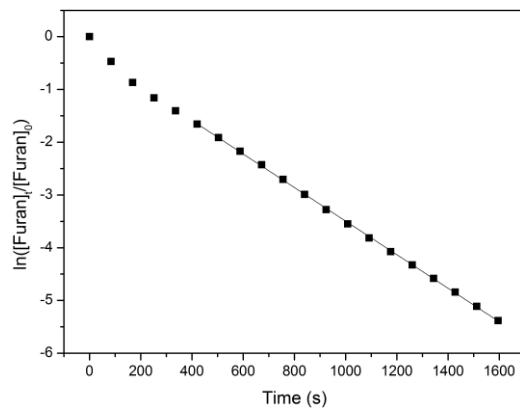
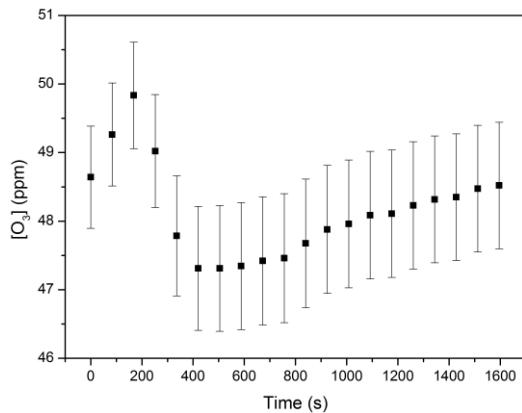
A.1 Furan

2013-04-16

2nd experiment



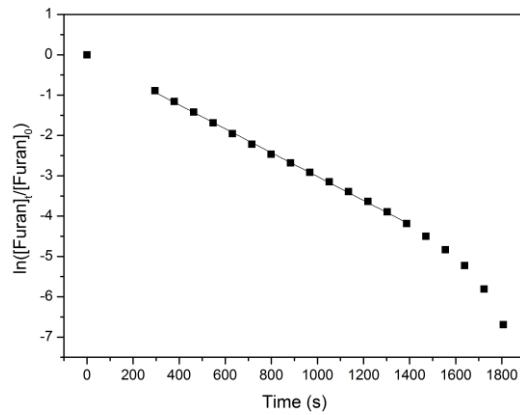
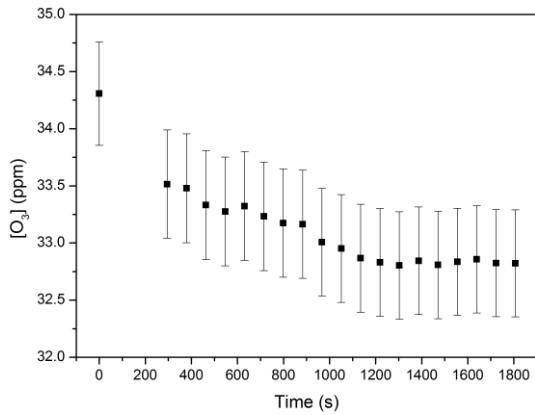
3rd experiment



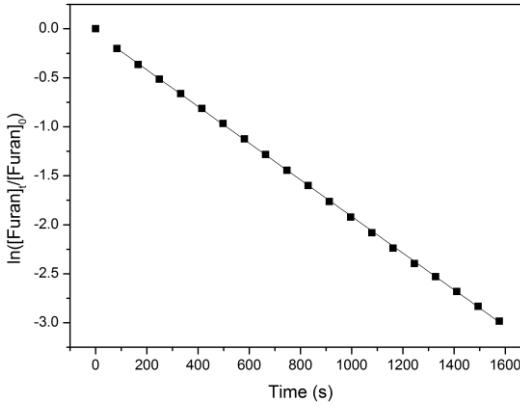
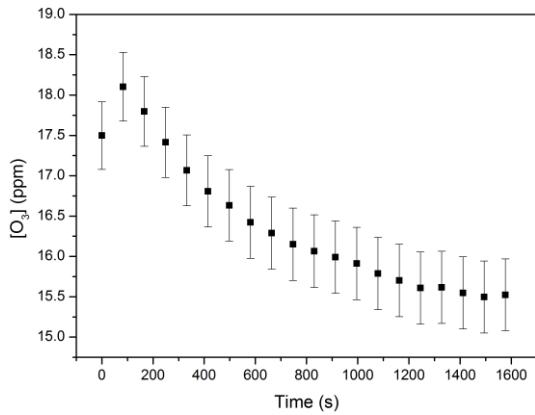
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2013-04-18

3rd experiment



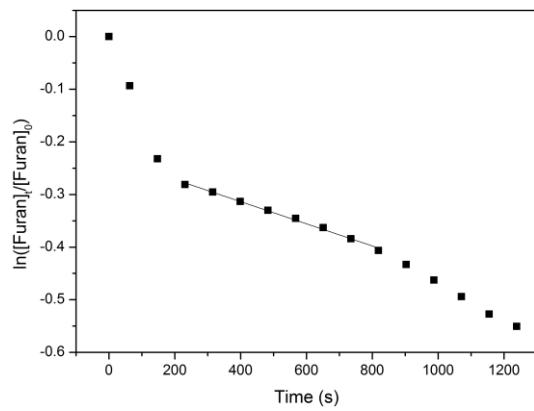
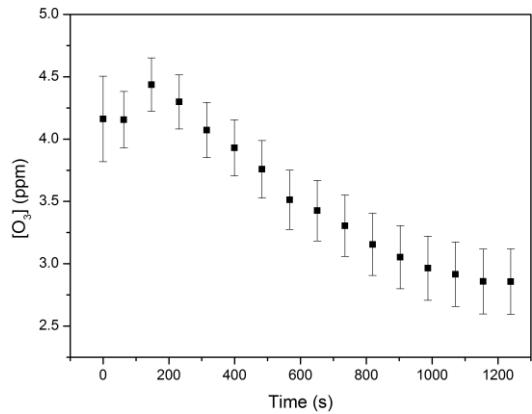
4th experiment



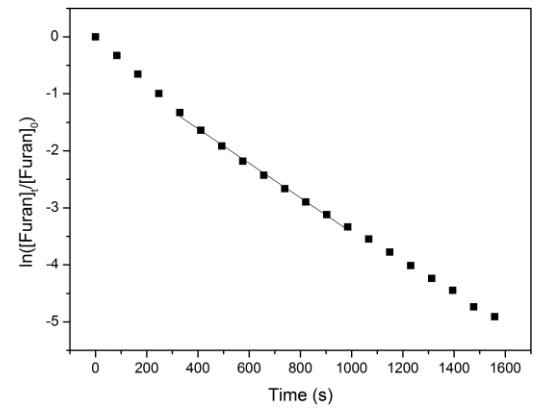
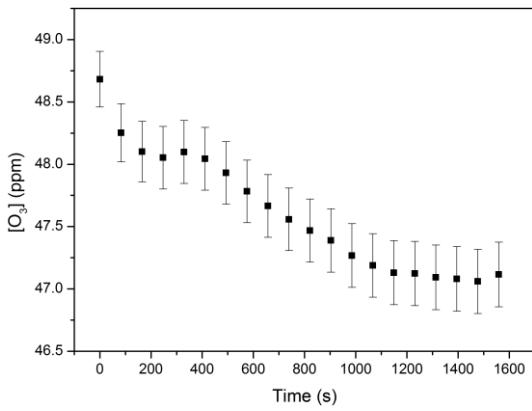
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2013-04-25

4th experiment

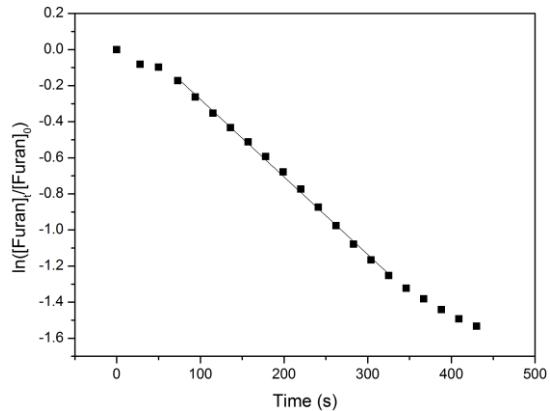
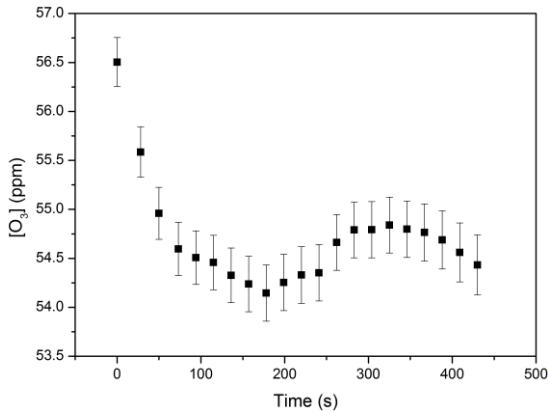


5th experiment

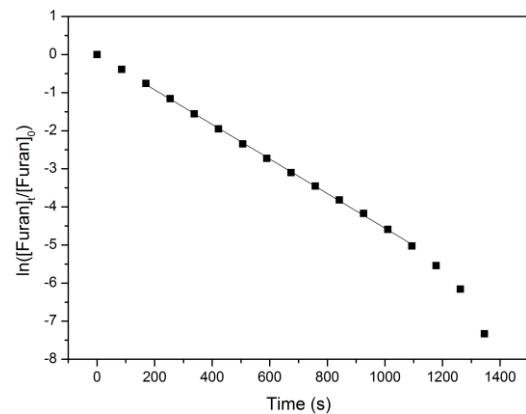
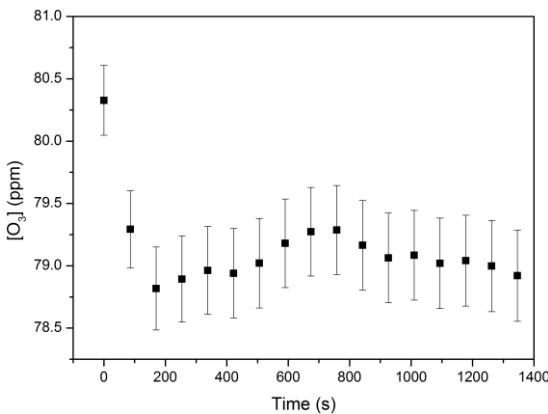


Furan - A Future Fuel and its Lifetime in Urban Air

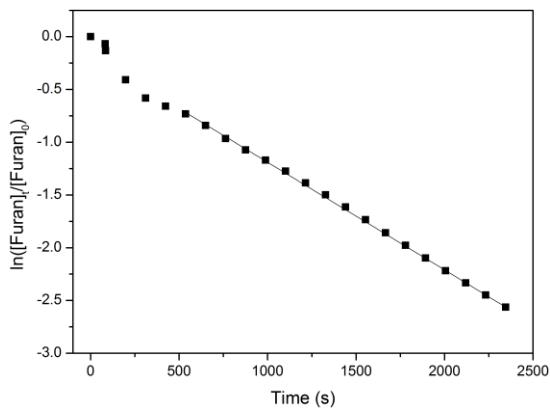
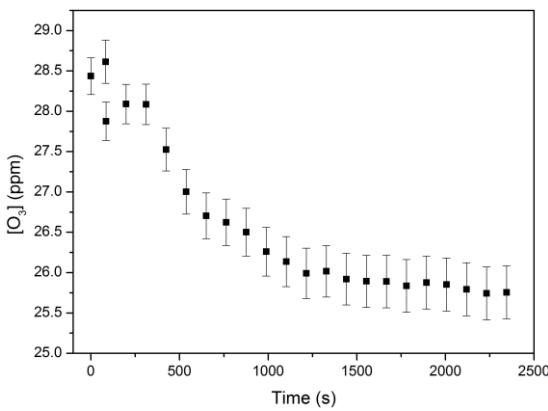
2013-04-26
3rd experiment



4th experiment

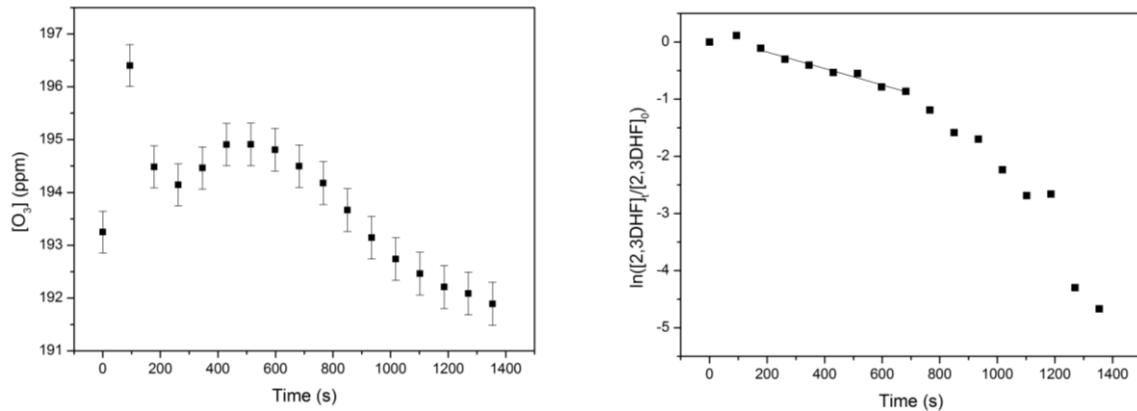


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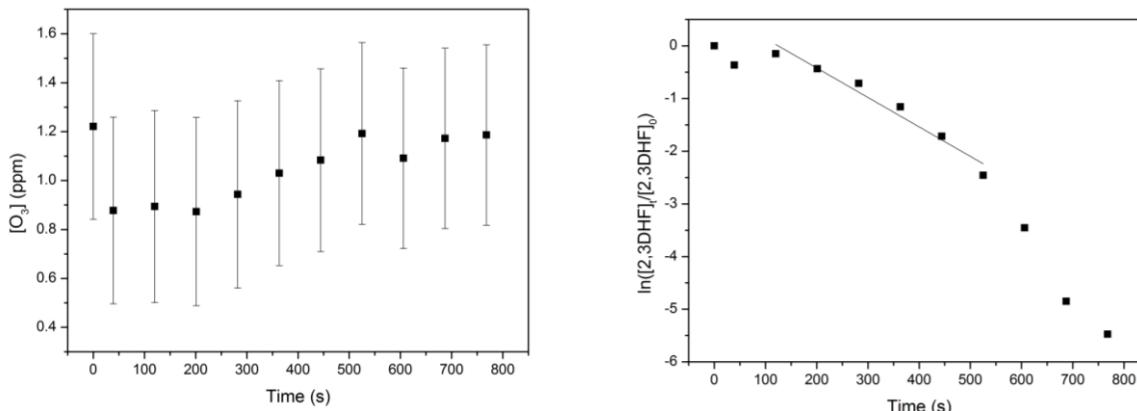


A.2 2,3 DHF

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2nd experiment

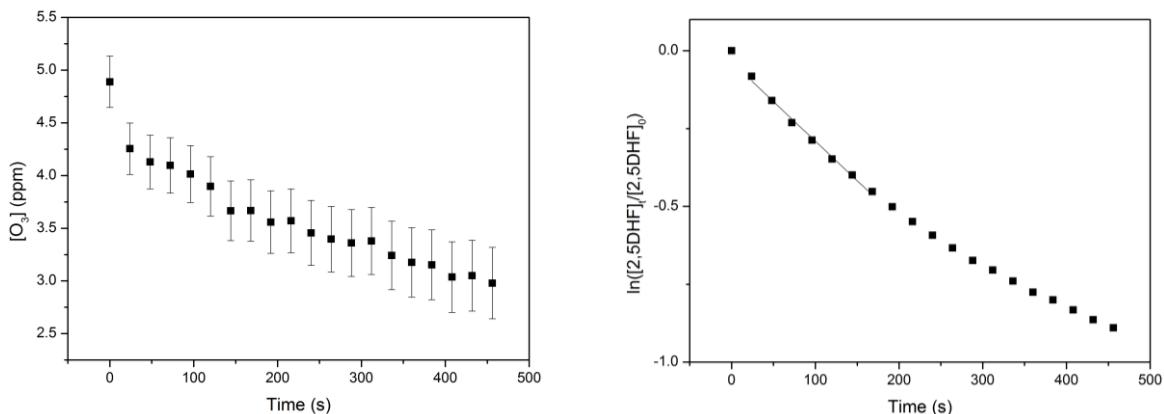


2013-04-25
2nd experiment



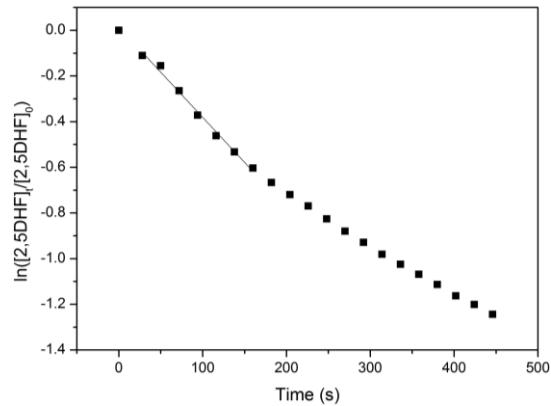
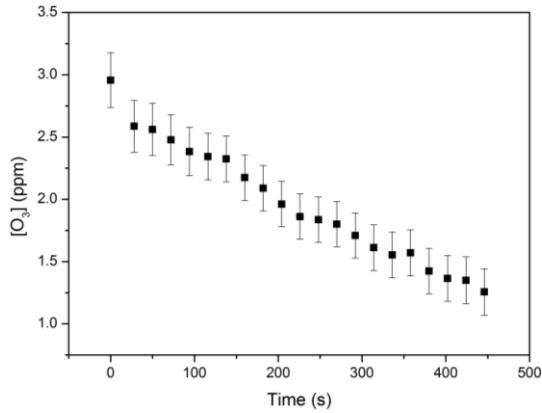
A.3 2,5 DHF

2013-04-22
7th experiment

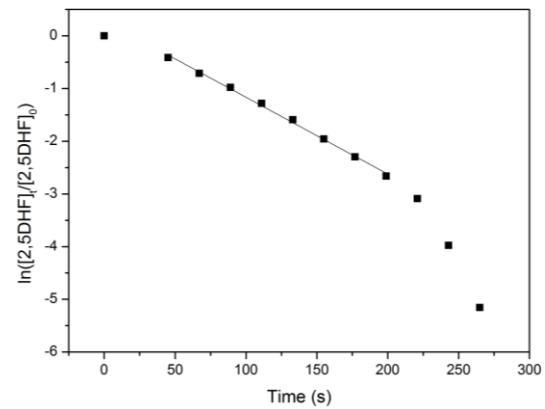
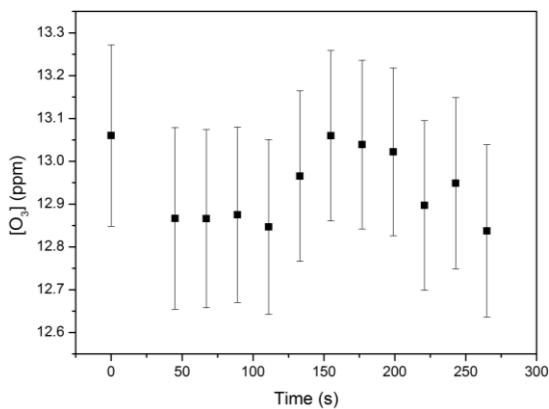


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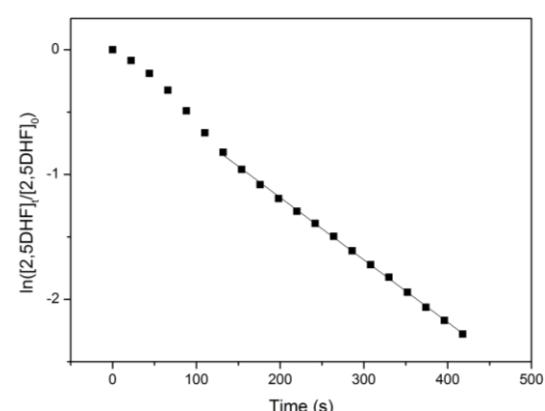
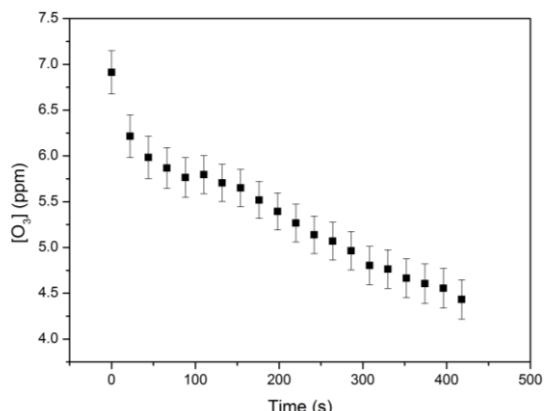
1st experiment



2nd experiment



3rd experiment



Appendix B

This appendix presents the essential properties of the three compounds investigated in the report above. It also contains a risk analysis for these compounds. Since the author of this report, also the one who performed the experiments, is Swedish the risk analyse are written in Swedish.

B.1 Physical properties of furan, 2,3- and 2,5 DHF

Table B1. Physical properties of Furan, 2,3-DHF and 2,5-DHF.

	Furan	2,3-DHF	2,5-DHF
Chemical name	C4H4O	C4H6O	C4H6O
Molecular weight	68,07 g/mol	70,09 g/mol	70,09 g/mol
Appearance (Form & Colour)	Liquid	Clear, Liquid Light brown	Liquid Yellow
Initial boiling point/ boiling range	32 °C at 1011 hPa – lit.	54-55 °C – lit.	66-67 °C – lit.
Flash point	- 36 °C closed cup	- 20 °C closed cup	1 ° C closed cup
Vapor pressure	635 hPa at 20 °C	996,7 hPa at 55 °C	252,9 hPa at 20 °C
Stability	Contains 0,025 % BHT		

B.2 Risk analysis

Furan

Furan är mycket brandfarlig och får därför inte utsättas för värme, flammor, gnistor, heta ytor eller direkt solljus, ämnet kan även bilda explosiva peroxider. Vid brand används släckmedel så som vattendimma, alkoholbeständigt skum, pulver eller koldioxid.

Furan ska förvaras väl tillsluten på sval, mörk, torr och väl ventilerad plats åtskild från antändningskälla. Rökning i anslutning till ämnet är strängt förbjuden! Öppnade behållare bör förvaras upprätt för att undvika läckage. Vid oavsiktligt utsläpp använd andningsskydd för att undvika att andas in ångan och säkerhetsställ god ventilation. Avlägsna alla antändningskällor och evakuera personalen. Ångor kan ansamlas lågt och bilda explosiva koncentrationer. Förhindra fortsatt läckage eller spill och utsläpp i avloppssystemet. Eftersom furan är mycket brandfarligt så bör försiktigheatsåtgärder vidtas då ämnet deponeras i förbränningssugn avsedd för kemikalier. Överskott lämnas till företag med tillstånd för avfallshantering.

Furan ska inte andas in eller förtäras, det irriterar hud, ögon, luftvägar och kan vid långvarig exponering orsaka cancer. Använd skyddsglasögon och tvätta alltid händerna innan rast och omedelbart efter hantering av ämnet. Långvarig hudexponering kan orsaka avfettning och dermatit. Ett viktigt symptom vid exponering är CNS-deppresion. Vid första hjälpen kontakta alltid läkare:

- Inandning, flytta personen till frisk luft. Vid andningsstillestånd ge konstgjord andning.
- Hudkontakt, tvätta med rikligt med tvål och vatten.
- Ögonkontakt, skölj rikligt med vatten.
- Nedsväljning, framkalla inte kräkning utan skölj munnen rikligt med vatten. Försök inte att ge en medvetlös person något via munnen.

2,3 DHF

2,3 dihydrofuran är mycket brandfarlig och får därför inte utsättas för värme, flammor, gnistor, heta ytor eller direkt solljus, ämnet kan även bilda explosiva peroxider. Vid brand bildas koloxider, använd släckmedel så som vattendimma, alkoholbeständigt skum, pulver eller koldioxid. Stora bränder släcks i största mån med stora mängder vatten i form av dimma eller spray. Använd vattenspray för att kyla oöppnade behållare.

2,3 DHF ska förvaras väl tillsluten på mörk, torr och väl ventilerad plats åtskild från antändningskälla. Rekommenderad förvaringstemperatur är 2-4 °C. Rökning i anslutning till ämnet är strängt förbjuden! Öppnade behållare bör förvaras upprätt för att undvika läckage. Vid oavsiktligt utsläpp använd andningsskydd för att undvika att andas in ångan och säkerhetsställ god ventilation. Avlägsna alla antändningskällor och evakuera personalen. Ångor kan ansamlas lågt och bilda explosiva koncentrationer. Förhindra fortsatt läckage eller spill och utsläpp i avloppssystemet. Eftersom 2,3 DFH är mycket brandfarligt så bör försiktighetsåtgärder vidtas då ämnet deponeras i förbränningssugn avsedd för kemikalier. Överskott lämnas till företag med tillstånd för avfallshantering.

2,3 DHF ska inte andas in eller förtäras och det irriterar både hud, ögon och luftvägar. Använd skyddsglasögon och tvätta alltid händerna innan rast och omedelbart efter hantering av ämnet. Viktiga symptom vid exponering är CNS-deppresion, narkos, hosta, andningssvårighet, illamående, yrsel, huvudvärk och medvetslöshet. Vid första hjälpen kontakta alltid läkare:

- Inandning, flytta personen till frisk luft. Vid andningsstillestånd ge konstgjord andning.
- Hudkontakt, tvätta med rikligt med tvål och vatten.
- Ögonkontakt, skölj rikligt med vatten.
- Nedsväljning, framkalla inte kräkning utan skölj munnen rikligt med vatten. Försök inte att ge en medvetlös person något via munnen.

2,5 DHF

2,5 dihydrofuran är mycket brandfarlig och får därför inte utsättas för värme, flammor, gnistor, heta ytor eller direkt solljus, ämnet kan även bilda explosiva peroxider. Vid brand bildas koloxider, använd släckmedel så som vattendimma, alkoholbeständigt skum, pulver eller koldioxid. Använd vattenspray för att kyla oöppnade behållare.

2,5 DHF ska förvaras väl tillsluten på sval, torr och väl ventilerad plats åtskild från antändningskälla. Rökning i anslutning till ämnet är strängt förbjuden! Öppnade behållare bör förvaras upprätt för att undvika läckage. Vid oavsiktligt utsläpp använd andningsskydd för att undvika att andas in ångan och säkerhetsställ god ventilation. Avlägsna alla antändningskällor och evakuera personalen. Ångor kan ansamlas lågt och bilda explosiva koncentrationer. Förhindra fortsatt läckage eller spill och utsläpp i avloppssystemet. Eftersom 2,5 DFH är mycket brandfarligt så bör försiktighetsåtgärder vidtas då ämnet deponeras i förbränningssugn avsedd för kemikalier. Överskott lämnas till företag med tillstånd för avfallshantering.

2,5 DHF ska inte andas in eller förtäras och det irriterar både hud, ögon och luftvägar. Tvätta alltid händerna innan rast och omedelbart efter hantering av ämnet. Vid första hjälpen kontakta alltid läkare:

- Inandning, flytta personen till frisk luft. Vid andningsstillestånd ge konstgjord andning.
- Hudkontakt, tvätta med rikligt med tvål och vatten.
- Ögonkontakt, skölj rikligt med vatten.
- Nedsväljning, framkalla inte kräkning utan skölj munnen rikligt med vatten. Försök inte att ge en medvetlös person något via munnen.