Open Access

Baghdad Science Journal **Vol.14(3)2017**

DOI: http://dx.doi.org/10.21123/bsj.2017.14.3.0547

Kinetic and Mechanistic Studies for the Gas-phase Reaction of Ozone with 2, 3-Dimethyl-2-Butene and 1, 3-Butadiene

Ismael Abdulsatar AL Mulla

Department of Chemistry, College of Science for Woman, University of Baghdad, Baghdad, Iraq.

E-mail: ismaelalmulla@yahoo.co.uk

Received 6/3/2017
Accepted 22/5/2017

Abstract:

The reactions of ozone with 2,3-Dimethyl-2-Butene $(CH_3)_2C=C(CH_3)_2$ and 1,3-Butadiene $CH_2=CHCH=CH_2$ have been investigated under atmospheric conditions at 298±3K in air using both relative and absolute rate techniques, and the measured rate coefficients are found to be in good agreement in both techniques used. The obtained results show the addition of ozone to the double bond in these compounds and how it acts as function of the methyl group substituent situated on the double bond. The yields of all the main products have been determined using FTIR and GC-FID and the product studies of these reactions establish a very good idea for the decomposition pathways for the primary formed compounds (ozonides) and give a good information for the effect of the methyl group on the degradation pathways. The results have been discussed from the view point of their importance in the atmospheric oxidation of these pollutants.

Key words: Ozone, reactions kinetics, absolute rate, relative rate, rate constant, reactivity, and reaction mechanism

Introduction:

In most of the countries, air pollution is considered as a major problem, particularly high levels of smoke and sulfur dioxide arising from the combustion of fossil fuels that contain sulfur. Pollution is the real threat to the air which caused by dangerous emissions of poisons and particles. This major problem comes from a fact that is petrol and diesel engine motor vehicles emit a wide variety of pollutants, principally carbon monoxide CO, oxides of nitrogen NOx, volatile organic compounds (VOCs) and particulates (PM10) those completely have increased the impact on urban air quality. Add to that, photochemical reactions that come as a result from the action of sunlight on nitrogen dioxide NO_2 and VOCs emits from vehicles, can definitely lead to the formation of ozone, which is considered as a secondary long-range pollutant, that impacts in rural areas that far from the original place of emission [1]. Most of the available measurements refer to another fact which is that VOCs have been noticed as a major component of the trace gases found in the troposphere [2, 3].

Many complicated chemical processes occurring in the atmosphere lead to the formation of ozone and some other photochemical pollutants [4]. All these processes participating in a very high percentage in formation of ozone, and many other chemical compounds like peroxyacetyl nitrate PAN nitric acid HNO_3, sulfuric acid H_2SO_4 particulate matter, formaldehyde (HCHO), and carbonyl compounds [5-7]. Because of a variety of complex VOCs emits to the atmosphere in very large quantities from both anthropogenic and biogenic sources which is itself a very complicated chemistry. The cycles of photochemical reactions lead to formation of ozone that can be best understood by studying and well understanding of the atmospheric oxidation of methane CH_4 [8]. In addition, there is evidence for the importance of chlorine atom reactions with various alkanes and alkyl nitrates in the arctic troposphere during springtime [9, 10].

1,3-butadiene, and 2,3-dimethyl-2-butene among those VOC emitted into the troposphere principally from many sources like fuel combustion and from refinery industry and biomass burning as well as many other sources of burning and forest fires [11,12]. However, the reactions of 1,3-Butadiene in the troposphere with OH radicals, NO_3 radicals, and O_3 can participate in the removal processes of 1,3-Butadiene from this layer. Because of OH high concentrations, its reaction with 1,3-Butadiene dominates in the atmosphere during the daytime, while the loss processes through the reactions with ozone and NO_3 still doing its part in the overall removal process of 1,3-Butadiene from the atmosphere. Acrolein and formaldehyde have been noticed as the initial products from those reactions and considerably furan from the reaction with OH, and nitrates from the reaction with NO_3 [5,11]. There were some studies suggested that a possible reaction of 2,3-dimethyl 2-butene with bromine may be participated in elimination of this compound from the atmosphere [13].

Materials and Methods:

All experiments have been carried out at 298±3 K in air and at atmospheric pressure in a Teflon reaction vessel of volume 50 L. The reaction vessel was based in a chamber. The reaction vessel was connected to a GC-FID system and FTIR spectroscopy analytical system by Teflon tubing. The relative rate, absolute rate kinetic studies and product distribution studies were well explained previously [14], where most of the experiments been carried out in Department of Chemistry Laboratories – University College Dublin (UCD), and in Department of Chemistry Laboratories – Dublin Institute of Technology (DIT).

The experimental and analytical systems employed in this work and the vacuum system consisted of a Pyrex high vacuum line fitted with Teflon® vacuum taps (J. Young Scientific Ltd). The vacuum was maintained by an Edwards rotary vane vacuum pump (model RV3) fitted with a liquid nitrogen cooled trap, and monitored by a Pirani gauge head (Edwards, model APG-L) connected to an Edwards AGD Pirani readout unit. The vacuum was typically in the region of $1x10^{-3}$ Torr, and reactant pressures were measured by two MKS Baratron capacitance manometers (model 626A 1-10 Torr and model 626A 1-1000 Torr) in conjunction with a two channel digital readout unit (MKS, model PR 4000). All quantitative analyses were carried out using a Shimadzu GC-14B with a flame ionization detector. While for the mechanism and product studies, FTIR spectrometer with detector of mercury cadmium telluride was used to analyze the reaction mixtures.

The materials employed in the kinetic investigations were synthetic air, zero-grade, 99.95% (Air Products), Air for GC (Laboratory air), JUN AIR (model 302-5S Products of Technology Ltd.). Nitrogen, 99.9995% (MicroGeN$_2$ – Products of Technology Ltd). Hydrogen for GC, 99.99999%, Matheson Chrysalis ^{TM} hydrogen generator (model GEN-HYC 300). 2,3-dimethyl-2-butene $(CH_3)_2C=C(CH_3)_2$, 99% (Sigma-Aldrich), 1,3-butadiene $CH_2=CHCH=CH_2$, 99% (Sigma-Aldrich). Some other materials were used for purposes of calibrations and OH radicals scavenging to get the reactions takes place for only materials with ozone, as well as for product confirmation 1-methylcyclohexene (1-CH3-C6H9), 97% (Sigma-Aldrich), Propene (CH2=CHCH3), 99% (Sigma-Aldrich), cyclohexane (c-C6H12), 99.9% (Sigma-Aldrich) and formic acid (HC(O)OH), 98% (Fluka). All materials were used as received. The reaction products, acetone $(CH_3)_2CO$, 99% (Aldrich) was used as received. In relative rate experiments, ozone have been generated by using ozone generator (Monitor Labs).

Results: Relative Rate Studies

The relative rate technique is well known as a reliable technique that has been used to study the gas-phase reactions of VOCs with O_3 and NO_3 [14, 15]. The results for relative rate coefficients for all the reactions of O_3 with the target compounds have been determined by comparing their decay rates with the decay rates of reference compounds which rate coefficients have been previously established. These results were based on the presence of ozone, the substrate (target compound under investigation) and reference compounds decay due to reactions (1) and (2).

$$O_3 + \text{Substrate} \xrightarrow{k_1} \text{Products} \qquad (1)$$

$$O_3 + \text{Reference} \xrightarrow{k_2} \text{Products} \qquad (2)$$

$$\frac{-d\ln[\text{Substrate}]}{dt} = k_1[O_3] \qquad (III)$$

$$\frac{-d\ln[\text{Reference}]}{dt} = k_2[O_3] \qquad (IV)$$

$$\frac{-d\,[\text{Substrate}]}{dt} = k_1\,[O_3]\,[\text{Substrate}] \qquad (I)$$

$$\frac{-d\,[\text{Reference}]}{dt} = k_2\,[O_3]\,[\text{Reference}] \qquad (II)$$

No any organic compound is reformed by any process, so both compounds are lost only by reaction with O_3 and negligent dilution quantity of O_3 due to sampling.

Eliminating O_3 concentrations gives,

$$\ln\left(\frac{[\text{Substrate}]_0}{[\text{Substrate}]t}\right) = \frac{k_1}{k_2}\ln\left(\frac{[\text{Reference}]_0}{[\text{Reference}]t}\right) \qquad (V)$$

where $[\text{Substrate}]_0$ and $[\text{Reference}]_0$ represent the concentrations of substrate and reference compounds, respectively at time 0, while $[\text{Substrate}]_t$ and $[\text{Reference}]_t$ represents the corresponding concentrations at time t, and k_1 and k_2 are the rate coefficients for reactions (1) and (2) respectively.

For the reactions of O_3 with 1,3-butadiene, and 2,3-dimethyl-2-butene, ozone was introduced by additions to the system during the course, because ozone was generated at time of the experiment, so it was introduced by pushing it into the reaction bag from the generator, and this continued in each experiment till the concentration of the target compound get nearly finished from the reaction bag. Each addition of ozone causes a kind of dilution for the concentration of the reactants in the system, with the dilution factor at time t being D_t, (where $D_t = \ln [C]_0 / [C]_t$ where C_0 and C_t are the concentrations of a chemically inactive species (zero air that pushed the ozone into the reaction bag and causes dilution) at time t_0 and t respectively). Hence, equation (V) can be changed to:

$$\ln \frac{[\text{Substrate}]_0}{[\text{Substrate}]t} - D_t = \frac{k_1}{k_2} \ln \frac{[\text{Reference}]_0}{[\text{Reference}]t} - D_t \qquad (\text{VI})$$

The concentrations of both target and reference compounds as a function of reaction time were plotted according to equation (VI) for reactions of O_3 and the slopes of the plots give the rate coefficient ratios k_1/k_2.

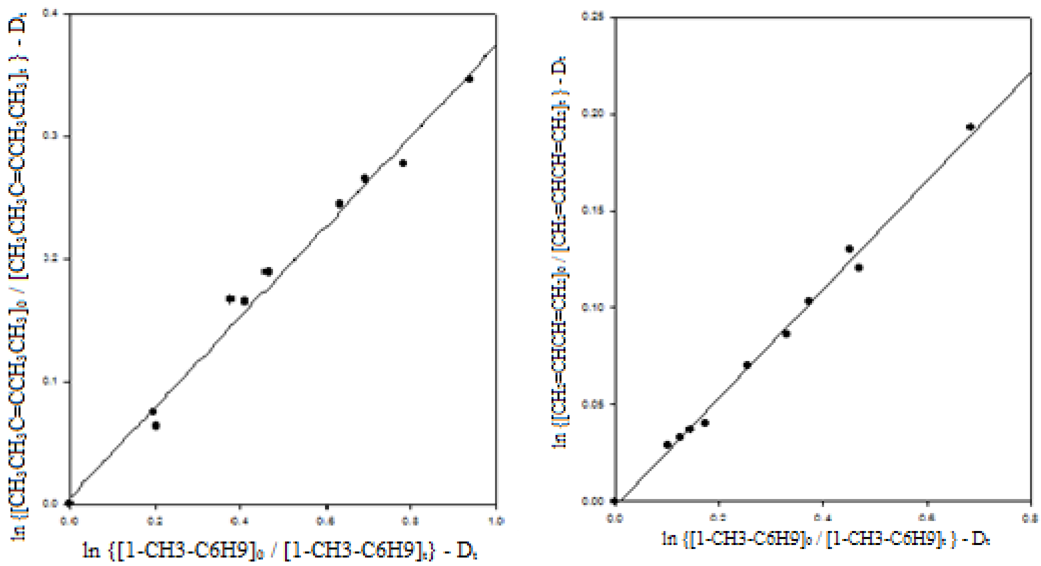


Fig.1: Concentration-time data for the reaction of O_3 with (a) 2,3-dimethyl-2-butene / 1-Methyl-1-cyclohexene, and (b) 1,3-butadiene / 1-Methyl-1-cyclohexene mixtures at 298 ± 2K and atmospheric pressure plotted depending on equation (VI).

The results obtained by this work shown in the table below:

Table 1: Averaged relative rate coefficients for the reaction of O_3 with 1,3-butadiene, and 2,3-dimethyl-2-butene **at 298 ± 2K and atmospheric pressures.**

Compound	Reference	k_1 / k_2 [(a)]	k_2 [(b, c)]	k_1 [(b)]
2,3-dimethyl 2-butene	1-Methyl-1-cyclohexene	1.31 ± 0.10	1.62×10^{-16}	$(2.12 \pm 0.15) \times 10^{-16}$
1,3-butadiene	1-Methyl-1-cyclohexene	2.11 ± 0.11	1.62×10^{-16}	$(3.41 \pm 0.19) \times 10^{-16}$

(a) In units of cm^3 $molecule^{-1}$ s^{-1}.

(b) Errors are twice the standard deviation and represent precision only; the error in the reference rate coefficient will add approximately 20 % to the uncertainty of the quoted rate coefficients.

(c) Taken from reference [16].

Absolute Rate studies

All the experiments were based on a technique that depends on measuring the loss of ozone molecules which considerably reacts with a known excess concentration of the reactant compound

(1,3-butadiene, and 2,3-dimethyl 2-butene). Background ozone decays where no oxygenated compounds present in the system been determined periodically and showed that negligible quantity of ($\leq 10^{-4}$ s^{-1}) compared to the loss rates of ozone where substrate compounds is presence.

All the absolute rate experiments were performed under the conditions of pseudo-first order conditions with $[Substrate]_0 >> [O_3]_0$. By monitoring the increased rates of ozone loss (decay) in the presence of known concentrations of the target compounds (substrate), second-order rate coefficients will be obtained. In the presence of the target molecule (substrate), the following processes remove ozone:

$$O_3 + \text{Substrate} \xrightarrow{k_3} \text{Products} \quad (3)$$

$$O_3 + \text{Wall} \xrightarrow{k_4} \text{loss of } O_3 \quad (4)$$

and hence

$$-d[O_3]/dt = (k_3[\text{Substrate}] + k_4)[O_3] \quad (VII)$$

where k_3 and k_4, are the rate coefficients for reactions (3) and (4) respectively.

Because the concentration of the target molecule (substrate) is in large excess, so it will remain essentially constant during the reaction, so the equation (VII) modified to:

$$-d\ln[O_3]/dt = k_3[\text{Substrate}] + k_4 \quad (VIII)$$

and $$[O_3]_t = [O_3]_0\, e^{-k^{`} t} \quad (IX)$$

where $$k^{`} = k_3[\text{Substrate}] + k_4 \quad (X)$$

The second-order rate coefficient k_3 can be obtained from the dependence of k\` (equation X: $k^{`} = k_3[\text{Substrate}] + k_4$) on the initial concentration of the target molecule (substrate), because we already found that the decay of ozone in reaction (4) is negligible compared to the loss rates of ozone due to the reaction with the substrate itself.

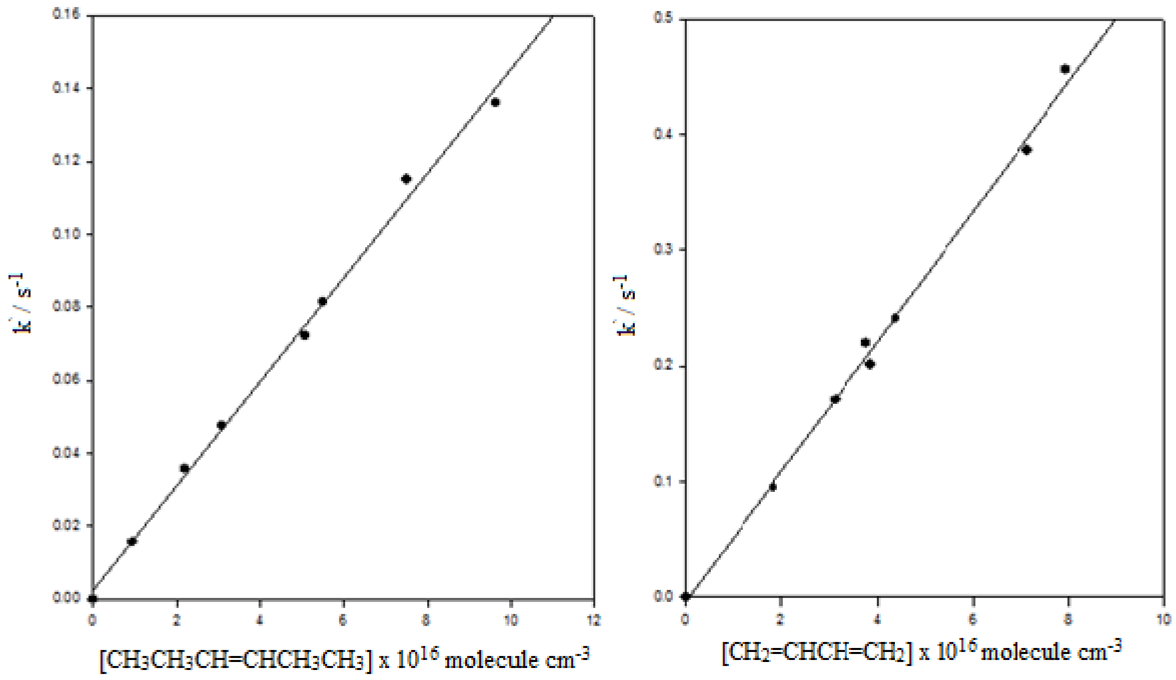

(a) (b)

Fig. 2: Plot of k\`/ s^{-1} versus (a) 2,3-dimethyl-2-butene $[CH_3CH_3CH=CHCH_3CH_3]$ / molecule cm^{-3} and (b) 1,3-butadiene $[CH_2=CHCH=CH_2]$ x 10^{16} molecule cm^{-3} for their reactions with O_3 at 298 ± 3K and atmospheric pressure.

The results been obtained by this work are shown in the table below:

Table 2: Averaged absolute rate coefficients for the reaction of O_3 with 1,3-butadiene, and 2,3-dimethyl-2-butene at 298 ± 2K and atmospheric pressure.

Compound	k_3 $^{(a,b)}$
2,3-dimethyl-2-butene	$(1.98 \pm 0.10) \times 10^{-16}$
1,3-butadiene	$(3.16 \pm 0.12) \times 10^{-16}$

(a) In units of cm^3 $molecule^{-1}$ s^{-1}.

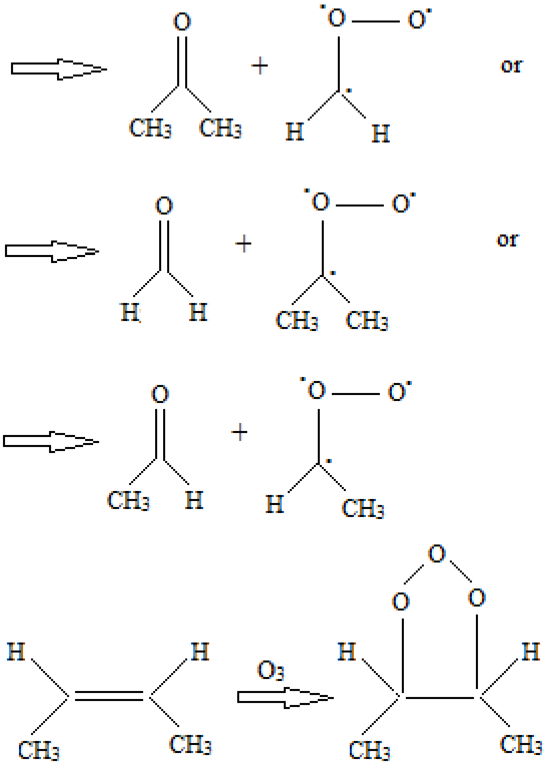
(b) Errors represent the precision only, and they are twice the standard deviation.

Discussions:

The reactions of ozone with an alkene always lead to breaking down of the C=C double bond and usually forms an aldehyde or ketones and carboxylic acids

1- For the reaction of 2,3-dimethyl-2-butene $(CH_3)_2C=C(CH_3)_2$ with ozone, the proposed pathway of this addition is to give the primary unstable compound (an ozonide), which rapidly suffering bond cleavage to different possible compounds, ketone, acetaldehyde, and unstable compound (Criegee biradical) which itself degrades further more as it is shown in scheme (1).

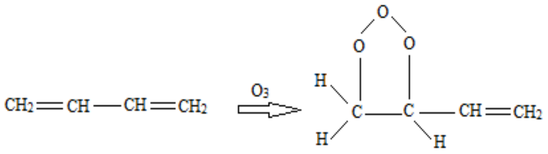
In the atmosphere, aldehydes (RCHO) and ketones (RC(O)R′) undergo different types of reactions (photolytic and chemical) and therefore they have been considered as key species. They live in the atmosphere till it gets further reactions and gets degraded into more simple compounds. Loss of ketones from the atmosphere is believed to be mainly due to reaction with OH radicals [17].



Scheme (1): Proposed mechanism for the reaction of ozone addition to 2,3-dimethyl-2-butene with the possible products and unstable compounds (Criegee biradical)

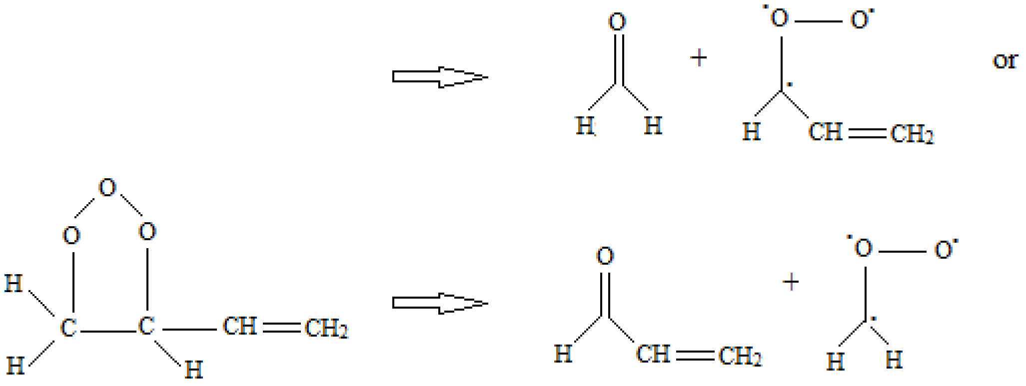
The reaction of an alkene molecule with the electrophilic ozone molecule can be enhanced by the electron-donating methyl group (CH_3) which substitutes the hydrogen atom in the alkene [15]. Therefore, once we have more methyl groups added to the alkene molecule, we simply can notice the clear effect on the reaction coefficient measured to that reaction. It is been clearly noticed that the successive methyl substitution of butene leads to increase in the rate of addition of the ozone molecule to the alkene double bond system. Decomposition of the ozonide mainly generates a ketone, or aldehyde and biradical. In this reaction, the cleavage of the π-bond is occurring through the dipolar addition, while the σ-bond cleavage is by rearrangement step of the reaction. Accordingly, both bonds of C=C unit of alkene been cleaved and further transformation of each carbon atom of the double bond system C=C can result in born of new C=O unit in forming aldehydes or ketones.

2- For the reaction of 1,3-Butadiene $CH_2=CHCH=CH_2$ with ozone, the proposed pathway of this reaction is to proceed as O_3 added identically to the double bond (for both sides of the compound) and gives the primary unstable compound (an ozonide as it shown in scheme (2a);



Scheme (2a): Proposed mechanism for the reaction of ozone addition to 1,3-Butadiene $CH_2=CHCH=CH_2$.

The ozonide then rapidly undergo identical cleavage to give possible products, formaldehyde or acrolein and the criegee biradical which itself decompose furthermore to more simple compounds (Scheme 2b);



Scheme (2b): Proposed cleavage mechanism for the unstable ozonide with the possible products

The acrolein oxidation in the atmosphere well be mentioned in the literature [18].

While the further atmospheric oxidation of the Criegee intermediate (CH_2OO) produced in mostly all the steps of the mechanisms suggested in this work is well studied and covered [19-21].

Conclusions:

The atmospheric lifetimes of the compounds investigated in this work due to removal by reaction with O_3 may be estimated from the measured rate coefficients. We can calculate the relative atmospheric lifetime for the compound of our interest with respect to its reaction with ozone by using the formula:

Lifetime $\tau O_3 = 1 / kO_3 [O_3]$

Where k_{O3} is the rate constant been calculated in this work, and $[O_3]$ is the tropospheric ozone concentration, (The averaged value of O_3 concentration for 24 hour been established to be = 7.0×10^{11} molecule cm^{-3}).

2,3-dimethyl-2-butene $(CH_3)_2C=C(CH_3)_2$ = 1.94 hrs. which is approximately 2 hrs.

1,3-Butadiene $CH_2=CHCH=CH_2$ = 1.21 hrs.

The calculated atmospheric lifetimes are only approximate values, since atmospheric concentration of ozone may vary significantly with season, location and time of day.

It has been noticed that the lifetimes values are relatively short, which indicates that if these compounds are present in the atmosphere, they will contribute and have a share in the formation of ozone in either local or regional areas because they will be degraded very soon after they get released into the troposphere.

Therefore, it has been suggested from this work that the obtained lifetime values with respect to the reaction with O_3 should be compared with the lifetimes values of the reactions of the same compounds with OH radicals, NO_3, bromine and chlorine atoms to determine which process is the faster removal process in the atmosphere.

It was hopped that the results of this work could be used by the dissection makers and the planners for the policies in order to reach a lower level of emissions, especially the compounds of interests.

Acknowledgement

This work is dedicated to the memory of Prof. Howard Sidebottom of University College Dublin (UCD).

The author would like to thank Department of Chemistry in University College Dublin UCD, where most of the experiments were been carried out, for the help and support.

Thanks to Dr. Jack Treacy of Dublin Institute of Technology DIT for his contribution and help to finish all the absolute rate experiments in DIT laboratory.

References:

[1]Ray, M. B.; 2000. Photodegradation of the Volatile Organic Compounds in the Gas Phase: A Review. Dev. Chem. Eng. Mineral Process, 8(5/6): 405-439.

[2]Singh, H.; Chen, Y.; Standt, A.; Jacob, D.; Blake, D.; Heikes, B.; and Snow, J. 2001. Evidence from the Pacific troposphere for large global sources of oxygenated organic compounds. Nature, (410): 1078.

[3]Zhou, Sh.; Barnes, I.; Zhu, T.; and Benter, T. 2012. Kinetic Study of Gas-Phase Reactions of OH and NO_3 Radicals and O_3 with iso-Butyl and *tert*-Butyl Vinyl Ethers. *J. Phys. Chem. A*, *116* (35): 8885–8892

[4]Perng, Ch..; C, I-Li.; Wang, I. and Chou, M. 2011. Ozonation of Odorous Compounds in Gases Emitted from Rubber Processing Industries, Aerosol & Air Quality Res, 11: 51–58,

[5]Atkinson, R. J. 1994. Gas phase tropospheric chemistry of organic compounds. J. Phys. Chem. Ref. Data, (Monograph 2): 1-216.

[6]Kesselmeier, J. and Staudt, M. 1999. Biogenic Volatile Organic Compounds (VOC): An Overview on Emission, Physiology and Ecology. J. Atmos. Chem. (33, 1): 23–88.

[7]National Research Council. 1991. Rethinking the Ozone Problem in Urban and Regional Air Pollution. National Academy Press, Washington.

[8]Atkinson, R.; and Arey, J. 2003. Gas-phase tropospheric chemistry of biogenic volatile organic compounds: a review. Atmospheric Environment. 37 Supplement (No. 2): S197–S219.

[9]Huang, Binbin.; Lei, Chao.; Wei, Chaohai.; and Zeng, Guangming. 2014. Chlorinated volatile organic compounds (Cl-VOCs) in environment-sources, potential human health impacts, and current remediation technologies. J. Environment Int. (71): 118–138

[10]Eleonora, Lo. V.; Francesco, F.; Jgor, A.; Umberto, G.; Paolo, C.; Martin, L. W.; and Michela, M. 2016. Non-Methane Volatile Organic Compounds in the Background Atmospheres of a Southern European Mountain Site (Mt. Cimone, Italy): Annual and Seasonal Variability.

Aerosol & Air Quality Res., 16: 581–592.

[11] Jaoui, M.; Lewandowski, M.; Docherty, K.; Offenberg, J. H.; and Kleindienst, T. E. 2014. Atmospheric oxidation of 1,3-butadiene: characterization of gas and aerosol reaction products and implications for PM2:5. J. Atmos. Chem. Phys. (14): 13681-13704.

[12] Copeland, G.; Ghosh, M. V.; Shallcross, D. E.; and Dyke, J. M. 2011. A study of the alkene-ozone reactions, 2,3-dimethyl 2-butene + O_3 and 2-methyl propene + O_3, with photoelectron spectroscopy: Measurement of product branching ratio and atmospheric implications. Phys. Chem. Chem. Phys. 13(39): 17461-73.

[13] Laine, Patrick L.; Sohn, Yoon. S.; Michael Nicovich, J.; Mckee, Michael. L.; and Wine, Paul, H. 2012. Kinetics of elementary steps in the reaction of bromine with 2,3-dimethyl-2-butene under atmospheric conditions. Int. J. of Chem. Kinet. (14,1): 13-26.

[14] AL Mulla, Ismael.; Mellouki, Abdelwahid.; Treacy, Jack.; Viera, Lisa.; Morris, Rebecca.; and Sidebottom, Howard. 2011. Kinetics and Mechanisms for the Reactions of Ozone with Unsaturated Oxygenated Compounds. J. Chem. Phys. Chem. (11): 4069-4078.

[15] Stewart, D. J.; Almabrok, S. H.; Lockhart, J. P.; Mohamed, O. M.; Nutt, D. R.; Pfrang, C.; and Marston, G. 2013. The kinetics of the gas-phase reactions of selected monoterpenes and cyclo-alkenes with ozone and the NO_3 radicals. Atmospheric Environment. (70): 227-235.

[16] Treacy, J.; Curley, M.; Wenger, J.; Sidebottom, H. J. Chem. Soc. Faraday. Trans. 1997, 93, 2877.

[17] Affiliated**,** E. J.; and Barnes, I. 2014. Daytime Atmospheric Chemistry of $C_4 - C_7$ Saturated and Unsaturated Carbonyl Compounds. The Handbook of Environmental Chemistry. (32): 53-103

[18] Cathelain, K.; Mevel, R.; Menon, S.; Blanquart, G.; and Shepherd, J. E. 2014. Ignition and chemical kinetics of acrolein-oxygen-argon mixture behind shock waves. Elsevier. Washington.

[19] Sheps, L. 2013. Absolute ultraviolet absorption spectrum of a Criegee intermediate CH_2OO. J. Phys. Chem. Lett. 4(24): 4201–4205.

[20] Liu, Y.; Bayes, K. D.; and Sander, S. P. 2014. Measuring rate constants for reactions of the simplest Criegee intermediate (CH_2OO) by monitoring the OH radical. J. Phys. Chem. A. 118(4): 741–747.

[21] Newland, M. J.; Richard, A. R.; Alam, M. S.; Vereecken, L.; Muoz, A.; Rodenas, M.; and Bloss, W. J. 2015. Kinetics of stabilised Criegee intermediates derived from alkene ozonolysis: Reactions with SO_2, H_2O and decomposition under boundary layer conditions. Phys. Chem. Chem. Phys. 17(6): 4076–4088.

دراسات حركية وميكانيكية لتفاعل الطور الغازي بين الاوزون وكل من المركب 3,2-ثنائي مثيل-2-بيوتين والمركب 3,1-بيوتادايين

اسماعيل عبد الستار الملا اسماعيل

قسم الكيمياء، كلية العلوم للبنات، جامعة بغداد، بغداد، العراق

البريد الالكتروني : ismaelalmulla@yahoo.co.uk

الخلاصة:

تم دراسة حركية وميكانيكية التفاعل الكيميائي بين كل من 2,3-Dimethyl-2-Butene و 1,3-Butadiene مع الاوزون O_3 تحت درجة حرارة 298 ± 3K وضغط جوي باستخدام طريقتي القياس المستخدمة لدراسة حركيات تفاعلات الغازات وهي طريقة قياس السرعة المطلقة وطريقة قياس السرعة النسبية وقد تم ايجاد نتائج قيمة ثابت السرعة للتفاعلات بقيم توافقية ومتطابقة تقريبا بين الطريقتين. كما اثبتت النتائج ان نشاطية المركبات الكيميائية المستخدمة في الدراسة نحو تفاعل اضافة الاوزون الى الاصرة المزدوجة في كل مركب تتناسب مع موقع مجموعة المثيل المتواجدة في المركب وقربها من الاصرة المزدوجة.

اما بالنسبة لدراسة ميكانيكية مسلك نواتج تفاعل اضافة الاوزون للمركبين فقد تم استخدام FTIR, GC-FID وقد اظهرت الدراسة مسلك التحلل للمركب الاولي (الوسطي) المتكون نتيجة اضافة الاوزون الى الاصرة المزدوجة، اثر مجموعة المثيل المعوضة في المركب على الناتج النهائي من هذا التفاعل. تم مناقشة النتائج واهميتها في الاكسدة الجوية التي من الممكن حدوثها لهذه المركبات كملوثات في الجو.

الكلمات المفتاحية: اوزون، حركيات التفاعلات، السرعة المطلقة، السرعة النسبية، ثابت السرعة، نشاطية التفاعل، ميكانيكية التفاعل.