

# Alexey Mayorov, Kandidat Nauk (PhD) Chemistry, MSc Applied Mathematics and Physics

## CURRICULUM VITAE

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Birth Date: 03.01.78

Marital Status: Married

Citizenship: Russian Federation

Language Proficiency: Russian (Native), English, French, German

## 1. EDUCATION

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- 2007 **Kandidat Nauk (PhD) in Chemistry**,  
Emanuel Institute of Biochemical Physics of Russian Academy of Sciences  
(<http://sky1.chph.ras.ru/>)
- 2002 **Master of Science in applied mathematics and physics**  
in the field of “Applied Mathematics and Physics”,  
Moscow Institute of Physics and Technology (State University) (<http://phystech.edu/>)
- 1999 **Bachelor of Science, in applied mathematics and physics**  
in the field of “Applied Mathematics and Physics”,  
Moscow Institute of Physics and Technology (State University) (<http://phystech.edu/>)

## 2. Research Experience

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**2007– Current: Senior Researcher**,  
Emanuel Institute of Biochemical Physics  
of Russian Academy of Sciences (IBCP  
RAS)

- Scientific research of ozone behaviour with organic and non-organic substances under different conditions, using methods of Quantum chemistry
- Participation in conferences, writing articles
- Supervising and scientific guidance of undergraduate, MSc, and post-graduate students

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**2002-2007: PhD Student**,

- Emanuel Institute of Biochemical Physics of RAS, and
- Institute of Problems of Chemical Physics of RAS

- Research in Quantum chemistry, Chemical kinetics. Supervisor: Boris E. Krisyuk, Prof., D.Sc. ([bkris@mail.ru](mailto:bkris@mail.ru))
- Research in Polymer Chemistry and Chemical Physics. Supervisor Anatoly A. Popov, Prof., D.Sc. ([popov@sky.chph.ras.ru](mailto:popov@sky.chph.ras.ru))
- Participation in conferences, writing articles
- Supervising and scientific guidance of undergraduate and MSc students

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<b>2001-2002: Master of Science Student,</b> <ul style="list-style-type: none"> <li>• Emanuel Institute of Biochemical Physics of RAS, and</li> <li>• Institute of Problems of Chemical Physics of RAS</li> </ul>	<ul style="list-style-type: none"> <li>• Research in Quantum-Chemical Calculation Methods &amp; Programs. Supervisor Boris E. Krisyuk, Prof., D.Sc. (<a href="mailto:bkris@mail.ru">bkris@mail.ru</a>)</li> <li>• Research in Mechanism of Interaction of Ozone and the Double Bond of Ethylene. Supervisor Anatoly A. Popov, Prof., D.Sc. (<a href="mailto:popov@sky.chph.ras.ru">popov@sky.chph.ras.ru</a>)</li> </ul>
<b>1999-2001 Master of Science Student,</b> The Human Genome Structure Information Centre of the Engelhardt Institute of Molecular Biology, RAS	<ul style="list-style-type: none"> <li>• C++ programming of the DNA analysis program. Supervisor Yuri P. Lysov, D.Sc. (<a href="mailto:lysov@eimb.ru">lysov@eimb.ru</a>)</li> </ul>
<b>1998-1999 Bachelor of Science Student,</b> Group of electron microscopy of the M.M. Shemyakin and Yu.A. Ovchinnikov Institute of bioorganic chemistry of RAS	<ul style="list-style-type: none"> <li>• Research in “Surface modification of highly oriented pyrolytic graphite and mica for investigation of biological objects using scanning probe microscopy”. Supervisor Victor Demin, Kandidat Nauk (<a href="mailto:vvdem@ibch.ru">vvdem@ibch.ru</a>)</li> </ul>

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### 3. Main Results

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I have developed a multi-stage calculation approach, which simplifies calculation of the potential energy surface and its critical points for the open-shell singlet biradical systems, where ozone is present. The algorithm subsequently applies more sophisticated quantum-chemical methods for calculation of critical points along the intrinsic reaction coordinate:

- As a first approximation of the potential energy surface, I use a simple single-reference open-shell method;
- Then, to get the optimised geometry of the reagents, the potential energy surface, the first and second derivatives, I use a simple multi-configurational method, which has enough capacity to calculate thermodynamic parameters, though is not adequate enough to take into account the static and dynamic correlation of electrons. At this stage thermodynamic parameters are calculated;
- Next, using methods that take into account the dynamic and static electron correlation in full, I use a point-wise refinement of the section of the potential energy surface along the intrinsic reaction coordinate. This enables us to obtain not only simple vertical energy correction, but also a horizontal shift in the saddle point, the latter determining the activation energy of the reaction. This horizontal correction, which might increase the required level of the activation energy of a reaction, has not been taken into account by other approaches.

Developing this approach in practice, I have studied the primary stage of the ozonation of the double (C=C) bond with different substituents (C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>3</sub>F, C<sub>2</sub>F<sub>4</sub>, cis-C<sub>4</sub>H<sub>6</sub>, trans-C<sub>4</sub>H<sub>6</sub>), different configurations, e.g. conjugated double bond (butadiene, allene), and triple (C≡C) bond (C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>F<sub>2</sub>, C<sub>2</sub>FH). I also applied this approach for the double bond deformed in buten-2. In all cases, dependence of the competition of two ozonation mechanisms was investigated. I discovered that at the first stage of ozonation of organic matters, there is competition between two mechanisms of ozonation: concerted

ozone addition via a symmetric transition state (Criegee mechanism) and non-concerted ozone addition via a singlet biradical transition state (DeMore mechanism). I have proven that the degree of competition depends on the chemical environment of the double bond and on its configuration. The developed approach enabled to achieve correlation between the experimental rate constants of ozonation reactions and the calculated ones. Furthermore, due to insufficient optimization of the saddle point, the calculated rate constants are always 2 to 20 times smaller than the experimental ones, which is a very good result for quantum chemical calculations.

During this work I conducted scientific supervision of a research group of undergraduate and post-graduate students. Under my supervision, the following BSc., MSc. and Kandidat degrees were granted:

- 2006: Vasily A. Ovchinnikov is granted the degree of Bachelor of Science, Moscow Institute of Physics and Technology (State University), Molecular and Biology Physics Department, Emanuel Institute of Biochemical Physics of RAS;
- 2008 Vasily A. Ovchinnikov is granted the degree of Master of Science, Moscow Institute of Physics and Technology (State University), Molecular and Biology Physics Department, Emanuel Institute of Biochemical Physics of RAS;
- 2008: Eldar A. Mamin is granted the degree of Bachelor of Science, Moscow Institute of Physics and Technology (State University), Molecular and Biology Physics Department, Emanuel Institute of Biochemical Physics of RAS;
- 2009 Margorita A. Valigun is granted the degree of Master of Science, Moscow Institute of Physics and Technology (State University), Molecular and Biology Physics Department, Emanuel Institute of Biochemical Physics of RAS;
- 2009: Alexey A. Permyakov is granted the degree of Bachelor of Science, Moscow Institute of Physics and Technology (State University), Molecular and Biology Physics Department, Emanuel Institute of Biochemical Physics of RAS;
- 2010 Eldar A. Mamin is granted the degree of Master of Science, Moscow Institute of Physics and Technology (State University), Molecular and Biology Physics Department, Emanuel Institute of Biochemical Physics of RAS;
- 2009: Elizaveta I. Denisenko is granted the degree of Bachelor of Science, Moscow Institute of Physics and Technology (State University), Molecular and Biology Physics Department, Emanuel Institute of Biochemical Physics of RAS;
- 2011: Alexey A. Permyakov is granted the degree of Master of Science, Moscow Institute of Physics and Technology (State University), Molecular and Biology Physics Department, Emanuel Institute of Biochemical Physics of RAS;
- 2011: Vasily A. Ovchinnikov is granted the degree of is granted the scientific degree of Doctor of Philosophy in Chemistry, in Emanuel Institute of Biochemical Physics of RAS.

#### 4. Progress achieved in research for last few years:

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##### ***4.1. 2008-2011: Institute of Problems of Chemical Physics of RAS and in Emanuel Institute of Biochemical Physics of Russian Academy of Sciences (IBCP RAS):***

The aim of this stage of research was to develop and test a calculating approach to strictly quantify the ozonolysis reaction rate constants, while previous approaches allowed only to compare the rate of ozonolysis of two ozonation mechanisms (Criegee and DeMore). To do so, I performed multi-reference calculations of ozonolysis by means of MCSCF and CASSCF, because the studied system, due to ozone presence, is a singlet biradical and requires a more precise geometry calculation. But this method does not allow to quantify the activation energy, because of its misestimation of the correlation interactions. Then I used MRMP2 corrections for all the points along intrinsic reaction coordinate of the MCSCF method, but this method does not allow to get first and second derivatives and is very cumbersome. I decided to use a combination of this method which enables to benefit from their strong sides and significantly eliminate their weak sides. Today with the help of the developed approach, I calculated the rate constant for the reaction of ozone with ethylene, butadiene, allen, acetylene, tetrafluoroethylene etc.

At the same time, I studied ozonolysis of chlorinated ethylene ( $C_2H_3Cl$ , cis,trans- $C_2Cl_2H_2$ , 1,1-dichloroethylene,  $C_2HCl_3$ ,  $C_2Cl_4$ ), together with my current PhD student Eldar Mumin. At the same time, I studied dependence of ozonolysis of the cis,trans-butene on its skeleton deformations; together with my student Vasiliy Ovchinnikov who defended his PhD thesis in the fall of 2011.

##### ***4.2. 2002-2007: Institute of Problems of Chemical Physics of RAS and in Emanuel Institute of Biochemical Physics of Russian Academy of Sciences (IBCP RAS):***

I decided to repeat all my previous calculations of the ozone+ethylene reaction, but using open-shell unrestricted methods, which were more appropriate to describe a biradical system, such as singlet biradical ozone. I constructed three point-wise potential energy surfaces of the singlet ozone addition to ethylene and found other nonsymmetrical saddle points, which corresponded to situations where a double bond is attacked by a side oxygen of ozone. So I showed by means of one-reference method the existence of DeMore mechanism. Misestimation of the correlation interaction of UHF and UMP2 surfaces does not let us to quantify the activation energy of the reaction. The next point of my work was to find such method to compare the reaction rate constants in Criegee and DeMore mechanisms. It was the DFT method – UB3LYP. After all, I managed to calculate the reaction rate constants of both mechanisms. However, the ratio of the constants shows, that Criegee ozonolysis of the ethylene is thousands times faster than DeMore ozonolysis. So I started to change substituents at the double bond of ethylene chemicals to change the double bond configuration to find the situation where DeMore mechanism would be much more faster than Criegee. I studied ozonolysis of tetrafluoroethylene ( $C_2F_4$ ), and it turned out that I was right. This reaction goes through DeMore mechanism. Then I calculated reaction rate constants of ozonolysis of acetylene ( $C_2H_2$ ) and hexafluoropropylene ( $F_3C-CF=CF_2$ ). As a result, I have shown that the ratio of the rate constants of reactions of the two mechanisms depends on the substituents at the double bond. In order to calculate the total rate constant for the ozonolysis, one should take into account both reaction mechanisms.

**4.3. 2001-2002: Institute of Problems of Chemical Physics of RAS and in Emanuel Institute of Biochemical Physics of Russian Academy of Sciences (IBCP RAS):**

The main purpose of the research was to understand if singlet ozone attacks double bond of ethylene (C<sub>2</sub>H<sub>4</sub>) symmetrically (Criegee mechanism) or asymmetrically (DeMore mechanism). There has been a delusion that ozonolysis goes only through concerted ozone addition via a symmetric transition state. By means of the Gaussian98 program at the computer center of the Chernogolovka Institute of Problems of Chemical Physics, I constructed two different point-wise potential energy surfaces of the first stage of the ethylene ozonolysis, using the methods: RHF and RMP2. At that time, there was no 3D graphics programs. So I wrote the C++ program with additional 3D module VTK (virtual toolkit) to display 3D potential energy surface and locate stationary saddle points. It was found out that close-shell, restricted calculations did not let to describe the DeMore mechanism.

**4.4. 1999-2001: The human genome structure information center of the Engelhardt Institute of Molecular Biology, RAS**

Researched different mathematics methods for analyzing DNA structure; wrote a C++ program to analyze genetic bank databases. For this, I studied biochemical genetic DNA; how genes are coded in DNA by means of nucleotides, explored approaches for barcoding and sequence identification; studied molecular genetic databanks and other available genetic resources on the Internet.

**4.5. 1998-1999 Group of electron microscopy, Shemyakin and Ovchinnikov Institute of bioorganic chemistry of the Russian Academy of Sciences**

The theme of my research was “Surface modification of highly oriented pyrolytic graphite and mica for investigation of biological objects using scanning probe microscopy”. I conducted DNA extraction for further immobilization of short DNA pieces on the mica and pyrolytic graphite. I tried various chemical methods to connect DNA to mica oriented pyrolytic graphite, and to make the DNA thicker for better resolution. To study and measure DNA, I used atomic force microscope, tunneling scanning microscope, and electronic microscope. The aim of the work was to achieve such sensitivity and resolution to distinguish difference between nucleotides A, T, G, C to be able to conduct DNA mapping.

## 5. SKILLS AND TECHNIQUES

### 5.1. *Scientific skills and techniques:*

- Calculations with different programs: PCGAMESS (FIREFLY), GAMESS US, GAUSSIAN, CFOUR.
- Visualization and analysis of the results by means of CHEMCRAFT, GaussView, ChemOffice.
- Calculation methods: single-reference: HF, MP2, MP4; single-reference semi empirical DFT: CPW91, B3LYP, PBE0, B3PW91, O3LYP etc.; single-reference Coupled-Cluster: ccsd, ccsdt, CR-EOMCCSD(T); single-reference CI: QCISD; multi-reference calculations within MCSCF, CASSCF, MRMP2, MCQDPT; methods of molecular dynamics: QM, MM, and hybrid QM/MM.
- Programming languages: C, C++, Pascal, Fortran

### 5.2. *Other skills and techniques:*

- Linux/FreeBSD/Unix/Microsoft Network Setup, Administration and Information Security. Database setup, administration and security – 3 year experience as a volunteer network administrator at the White Sea Biological Station Department of Biology Lomonosov Moscow State University (2009-2011). Supervisor: Prof. Alexander Tzetlin ([abtzetlin@wsbs-msu.ru](mailto:abtzetlin@wsbs-msu.ru))

## 6. GRANTS AND AWARDS

- 2007 - Second Place Award at the XXV All-Russian School of Young Scientists Symposium on Chemical Kinetics. Department of Chemistry, Moscow State University.

## 7. PUBLICATIONS (IN CHRONOLOGICAL ORDER):

1. Oleg B. Gadzhiev, Stanislav K. Ignatov, Boris E. Krisyuk, **Alexey V. Maiorov**, Shruba Gangopadhyay, and Artem E. Masunov, Quantum Chemical Study of the Initial Step of Ozone Addition to the Double Bond of Ethylene, Oleg B. Gadzhiev \*†, Stanislav K. Ignatov †, Boris E. Krisyuk \*‡, Alexey V. Maiorov §, Shruba Gangopadhyay , and Artem E. Masunov, J. PHYS. CHEM. A, 2012, 116 (42), pp 10420–10434

The mechanisms of the initial step in chemical reaction between ozone and ethylene were studied by multireference perturbation theory methods (MRMP2, CASPT2, NEVPT2, and CIPT2) and density functional theory (OPW91, OPBE, and OTPSS functionals). Two possible reaction channels were considered: concerted addition through the symmetric transition state (Criegee mechanism) and stepwise addition by the biradical mechanism (DeMore mechanism). Predicted structures of intermediates and transition states, the energies of elementary steps, and activation barriers were reported. For the rate-determining steps of both mechanisms, the full geometry optimization of stationary points was performed at the CASPT2/cc-pVDZ theory level, and the potential energy surface profiles were constructed at the MRMP2/cc-pVTZ, NEVPT2/cc-pVDZ, and CIPT2/cc-pVDZ theory levels. The rate constants and their ratio for reaction channels calculated for both mechanisms demonstrate that the Criegee mechanism is predominant for this reaction. These results are also in agreement with the experimental data and previous computational results. The structure of DeMore prereactive complex is reported here for the first time at the CCSD(T)/cc-pVTZ and CASPT2/cc-pVDZ levels. Relative stability of the complexes and activation energies were refined by single-point energy calculations at the

CCSD(T)-F12/VTZ-F12 level. The IR shifts of ozone bands due to formation of complexes are presented and discussed.

2. B. E. Krisyuk, **A. V. Maiorov**, Quantum chemical study of the primary step of ozone addition at the double bond of ethylene, *KINETICS AND CATALYSIS*, Volume 52, Number 6, 798-804, 2011.

The mechanism of the primary step of the interaction between ozone and the double bond of ethylene has been investigated by various methods of quantum chemistry (MP2, QCISD, CCSD, MRMP2) and density functional theory (PBE0, OPTX, CPW91, B3PW91, OLYO, B3LYP, BLYP). The kinetics of two reaction pathways, namely, concerted ozone addition via a symmetric transition state (Criegee mechanism) and nonconcerted ozone addition via a biradical transition state (DeMore mechanism) has been calculated. Both mechanisms are describable well in the single-determinant approximation by the QCISD, CCSD, B3LYP, and PBE0 methods and in the multideterminant approximation by the MRMP2 method. The other methods are less suitable for solving this problem. The calculated data demonstrate that the reaction proceeds via both competing pathways. Rate constant values consistent with experimental data and plausible Criegee-to-DeMore rate constant ratios have been obtained. The concerted addition of ozone to ethylene is significantly more rapid than the nonconcerted addition.

3. B. E. Krisyuk, **A. V. Maiorov**, E. A. Mamin and A. A. Popov, 1. Effect of the deformation of the double bond in chlorinated ethylene on the rate and mechanism of the reaction with ozone, *RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY B, FOCUS ON PHYSICS*, Volume 5, Number 3, 465-473, 2011.

The reactivity of the strained C=C bond of the 1-chloroethylene molecule in the reaction with ozone was studied using ab initio (MP2, CASSCT, MRMP2) and DFT (B3LYP) calculations in conjunction with the 6-31+G\*\* basis set. The mechanisms of concerted and nonconcerted addition were examined. The strain  $\epsilon$  was introduced into the problem by changing the length of the C=C bond and specifying it as a non-optimized coordinate. It is shown that, at least at  $\epsilon \leq 2\%$ , the activation energy  $E_a$  decreases linearly with increasing strain. The sensitivities of both channels of the reaction to the strain are similar and only slightly dependent on the method of calculation. The results are analyzed within the framework of a previously developed approach, which makes it possible to obtain an analytical dependence of  $E_a$  on the force and to relate the change in  $E_a$  during deformation to the length and rigidity of the initial and transition states.

4. B. E. Krisyuk and **A. V. Maiorov**, Competition between the concerted and nonconcerted addition of ozone to a double bond, *RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY B, FOCUS ON PHYSICS*, Volume 5, Number 5, 790-796, 2011

Quantum chemistry methods are used to investigate the mechanism of the reaction of ozone with the double bond of ethylene. It is shown that there are two possible reaction mechanism; concerted addition through a symmetrical transition state (Criegee mechanism) and nonconcerted addition through a biradical transition state (DeMore mechanism). In the single-determinant approximation, both mechanisms were described by using the QCISD, CCSD, and B3LYP methods. These methods give a reasonable ratio between the rates of the two reaction channels, with the rate constants being closer to the experiment when calculated by the CCSD and B3LYP methods. Multiconfiguration calculations are performed at the MRMP2 level. They also show the presence of both channels of the reaction and yield reasonable values of the rate constants for reaction channels and the ratio thereof. It is shown that the reaction of ethylene with ozone via the concerted addition mechanism is much faster.

5. B. E. Krisyuk, **A. V. Maiorov**, V. A. Ovchinnikov, A. A. Popov, Quantum-chemical modeling of the route of the reaction of butene-2 with ozone. *Butlerov Communications*. 2011. Vol.28. No.17. P.11-16.

6. B.E. Krisuyk, **A.V. Maiorov**, V. A. Ovchinnikov, A.A. Popov., Effect of deformation on the reactivity of C=C bonds in reactions with ozone, *Journal of Characterization and Development of Novel Materials*, Volume 2, Num 3/4, Nova Science Publishers, Inc. New York. P., 363-373
7. B.E. Krisuyk, **A.V. Maiorov**, E.A. Mamin, A.A. Popov, The influence of chlorine atoms in chlorinated ethylene on the mechanism and rate of its reaction with ozone. *Journal of Characterization and Development of Novel Materials*, 2011, v.2 Num.3/4, Nova Science Publishers, Inc. New York. P. 385-396
8. V. A. Ovchinnikov, B. E. Krisuyk, **A. V. Maiorov**, E. A. Mamin, A. A. Popov, The influence of substituents at the double C = C bond in the mechanism of adherence of ozone, *Butlerov Communications*. 2011. Vol.25. №.5. P.45-51
9. B. E. Krisuyk, **A. V. Maiorov**, V. A. Ovchinnikov and A. A. Popov, The influence of deformation on the reactivity of C=C bonds in reactions with ozone, *RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY B, FOCUS ON PHYSICS*, Volume 4, Number 5, 734-741, 2010

The influence of strain in the reaction center containing a double bond on double bond reactivity at the first stage of the reaction with ozone was studied by the B3LYP density functional theory method and ab initio MP2, CCSD, QCISD, and MRMP2 multireference methods. The 6-31+G\*\* and 6-311+G\*\* basis sets were used. The reactions of ozone with ethylene and butylene were studied. Deformation ( $\epsilon$ ) was introduced by using the C=C bond length or the distance between extreme carbon atoms as a coordinate not subjected to optimization. Stretching of the double bond was found to activate the reaction by the mechanisms of symmetrical and nonsymmetrical addition. The sensitivities to deformation were similar in the two channels. When the butene fragment as a whole was stretched, a different picture was observed, and the reaction with ozone was decelerated. In both cases, the logarithms of rate constants linearly depended on  $\epsilon$ . The calculation results were analyzed using the approach developed earlier, which allowed the calculation results to be used to obtain an analytic form of the dependence of activation energy  $E_a$  on the strength of bonds and to relate deformation-induced changes in  $E_a$  to the length and rigidity of the initial and transition states.

10. B. E. Krisuyk, **A. V. Maiorov**, E. A. Mamin and A. A. Popov, Effect of chlorine atoms in chlorinated ethylene on the rate and mechanism of its reaction with ozone, *RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY B, FOCUS ON PHYSICS*, Volume 4, Number 5, 726-733, 2010

The UQCISD, UB3LYP, UMP2, and MRMP2 methods in conjunction with the 6-31+G\*\*/6-311+G\*\* and aug-cc-PVDZ basis sets are used to study the primary reaction of ozone with chlorinated ethylene derivatives: tetrachloroethylene, trichloroethylene, 1,2-trans-dichloroethylene, 1,2-cis-dichloroethylene, 1,1-dichloroethylene, and chloroethylene. The reaction is studied for both concerted and nonconcerted ozone addition. The UB3LYP DFT method in conjunction with the 6-31+G\*\* basis set is used to examine various modes of addition of ozone to these chlorinated ethylenes by the Criegee and DeMore mechanisms. The geometry and energy of the transition states, the enthalpy and entropy, and the rate constants and ratios thereof for all the reactions are calculated. The UB3LYP method generally satisfactorily describes the two reaction pathways and, largely correctly predicts the rate constants, in agreement with the available experimental data. At the same time, this method appears to be inapplicable to modeling the interaction of ozone with 1,1-dichloroethylene. In this case, the single-determinant approximation turns out to be unsuitable, and, therefore, MCSCF methods should be used. The MRMP2 method yields reasonable values of the rate constants for the DeMore mechanism, whereas in the case of the Criegee mechanism, the MP2 method does well. The UB3LYP/6-31+G\*\* and UQCISD/aug-cc-PVDZ methods give similar values of the



ratio between the rate constants for the two pathways, a result that demonstrates the versatility of the first one.

11. **A. V. Maiorov**, B. E. Krisyuk and A. A. Popov, The mechanism of ozone addition to acetylene, *RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY B, FOCUS ON PHYSICS* Volume 2, Number 1, 67-70, 2008

The primary stage of the reaction between ozone and acetylene was studied by the HF, MP2, and B3LYP quantum-chemical methods using the 6-31G family of basis sets and the aug-cc-pVDZ basis set. The formation of the transition state was shown to be preceded by the formation of a complex. Subsequently, the reaction could occur as concerted (the Criegee mechanism) or nonconcerted (the DeMore mechanism) addition. The geometry and energy of transition states, the entropy and enthalpy of activation, and rate constants were calculated for both reaction paths. It was shown that there was a competition of the Criegee and DeMore mechanisms, and the fraction of the reaction along the nonconcerted addition channel was 1–10%. The UB3LYP method was found to be the most suitable for solving this problem in the one-determinant approximation

12. **A. V. Maiorov**, B. E. Krisyuk and A. A. Popov, The reaction of ozone with hexafluoropropylene: Competition of concerted and nonconcerted addition, *RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY B, FOCUS ON PHYSICS*, Volume 2, Number 5, 707-710, 2008

The initial stage of the reaction between ozone and hexafluoropropylene (HFP) was studied by the DFT/B3LYP quantum-chemical method using the family of 6-31G basis sets and the cc-pVDZ+ basis set. Two reaction paths were compared, concerted (the Criegee mechanism) and nonconcerted (the DeMore mechanism) addition. For both reaction paths, the geometry and transition state energies, entropy, and thermodynamic and electronic enthalpy were calculated and the rate constants of the reaction were estimated. It was shown that the DeMore mechanism should be given preference for the reaction of HFP with ozone. UB3LYP calculations for the DeMore mechanism give reaction rate constants close to the experimental values.

13. **A. V. Maiorov**, B. E. Krisyuk and A. A. Popov, The interaction of ozone with tetrafluoroethylene, *RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY B, FOCUS ON PHYSICS*, Volume 26, Number 7, 22-26, 2007

14. B. E. Krisyuk, **A. V. Maiorov**, Popov A. The reaction of ozone with ethylene: a consistent or inconsistent adherence, *RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY B, FOCUS ON PHYSICS*, Volume 26, Number 6, 16-22, 2007

15. B. E. Krisyuk, **A. V. Maiorov**, Popov A. Quantum-chemical investigation of the mechanism of the reaction of ozone with ethylene, *RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY B, FOCUS ON PHYSICS*, Volume 22, Number 9, 3-9, 2003

## 8. SELECTED ABSTRACTS:

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Over the past ten years I have made over 36 oral presentations at national and international conferences, as well as more than 28 poster presentations. The abstracts are available on request.

1. **A. V. Maiorov**, B. E. Krisyuk, A. A. Popov, Effect of conjugated double bonds on the rate and mechanism of ozonolysis. Quantum-chemical study, XI INTERNATIONAL CONFERENCE FOR YOUNG SCIENTISTS "BIOCHEMICAL PHYSICS" AND SCHOLL "MODERN PROBLEMS OF BIOCHEMICAL PHYSICS", Institute of Biochemical Physics Russian Academy of Science, Moscow, Russia, 9 – 11 November, 2011.
2. **A. V. Maiorov**, Quantum-chemical study of the mechanisms of competition and Kriege ozonolysis of conjugated and nonconjugated Demura systems on the example of propylene, acrolein, acrylic acid, allene, and allyl alcohol, Proceedings of XVIII International Conference of Students and young scientists "Lomonosov-2011", Department of Chemistry, Moscow State University, 11 – 15 April, 2011, [http://lomonosov-msu.ru/archive/Lomonosov\\_2011/structure\\_32\\_1353.htm](http://lomonosov-msu.ru/archive/Lomonosov_2011/structure_32_1353.htm)
3. **A. V. Maiorov**, V. A. Ovchinnikov, B. E. Krisyuk, A. A. Popov, The study of competition and the mechanisms of ozonolysis Kriege Demura conjugated and nonconjugated systems on the example of propylene, acrolein, acrylic acid, allene, and allyl alcohol by methods of quantum chemistry, Abstracts of the XXIII International Winter Youth Scientific School "Perspective directions of Physico-Chemical Biology and Biotechnology", Moscow, 7-10 February 2011, M.M. Shemyakin and Yu.A. Ovchinnikov Institute of bioorganic chemistry of the Russian Academy of Sciences.
4. V. A. Ovchinnikov, B. E. Krisyuk, **A. V. Maiorov**, A. A. Popov, The calculation of multiconfiguration methods ozonolysis reaction of the deformed and undeformed cis- and trans-2-butene, Abstracts of the All-Russian Youth Conference "Achievements of Chemical Physics", Chernogolovka, 21-23 June 2011, page 42.
5. B. E. Krisyuk, **A. V. Maiorov**, E. A. Mamin, A. A. Popov, The influence of the substituent at the double bond and its deformation in a chlorinated ethylene in the reaction with ozone, VI All-Russian Conference-School "highly reactive intermediates of chemical and biochemical reactions", Moscow Region., Boarding house "Youth", 10-13 October 2011, page 27;
6. B. E. Krisyuk, **A. V. Maiorov**, E. A. Mamin, A. A. Popov, Comparison of multiconfiguration quantum-chemical methods of the primary stage of ozonolysis of ethylene, tetrafluoroethylene, and monochloroethylene, XXIII Symposium "Modern Chemical Physics", Tuapse, boarding house "beacon", September 23 - October 4, 2011, page 92
7. **A. V. Maiorov**, V. A. Ovchinnikov, B. E. Krisyuk, A. A. Popov, Description of the primary phase ozonolysis of ethylene and n-butene by various methods of quantum chemistry., Proceedings of XIV Youth Conference on Organic Chemistry, May 10-14, Ekaterinburg-2011, page 167.

## 9. PATENTS:

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"NONE"

