

Summary of Ph.D. Thesis

**Experimental and Modelling Studies on the Reactions of
the Sulfate Ion Radical**

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I. Introduction and objectives

Sulfur dioxide (SO₂) is a gaseous compound that accumulates in the atmosphere by volcanic activity and from anthropogenic sources such as combustion of fossil energy carriers. SO₂ is harmful to human health, direct exposure to higher levels of sulfur dioxide induces respiratory irritations.

On a global level, the major consequence of atmospheric SO₂ is the formation of acid rain or acid deposition. The pH of rainwater decreases significantly due to the formation of sulfuric acid according to Eq. 1, the *autoxidation* of hydrated SO₂. Autoxidation is a generic term for the reactions where the reductant is oxidized by elementary oxygen from air. The prefix ‘auto’ refers to the fact that the oxidant is seldom added deliberately in these processes but is simply taken up from the environment.



Autoxidation of SO₂ drew considerable attention from inorganic chemists, and detailed mechanistic studies revealed that the intermediates of the autoxidation process are of radical nature (mainly SO₃^{•-}, SO₄^{•-}, SO₅^{•-}).

Sulfate ion radical (SO₄^{•-}) is one of the most broadly studied free radicals in the literature, along with hydroxyl radical (OH[•]). SO₄^{•-} is a highly reactive transient species with strong oxidizing power $E^0(\text{SO}_4^{\bullet-}/\text{SO}_4^{2-}) = 2.43 \text{ V}$.

Beside its role in atmospheric oxidation chemistry, SO₄^{•-} is considered to be an oxidant in so-called advanced oxidation processes (AOPs) in water and wastewater treatment, and also has biochemical relevance, such as footprinting of protein oxidation.

The present thesis is dedicated to shed further light on the role of sulfate ion radical in the transition metal catalyzed and the iodide ion catalyzed, photoinitiated autoxidation of hydrated SO₂, and more generally, the autoxidation of S(IV). Traditional methods of aqueous solution kinetics are employed, as well as the laser flash photolysis technique for the direct observation of SO₄^{•-}. Computational simulations are carried out to study the potential effect of diffusion and spatial inhomogeneities during laser flash photolysis experiments.

II. Instrumentation and computation

The autoxidation kinetics of S(IV) was studied primarily by **UV-vis spectrophotometry**, using a Perkin Elmer Lambda 2S or a Perkin Elmer Lambda 25 scanning spectrophotometer. Kinetic experiments were carried out in standard quartz cuvettes (optical path length = 1.000 cm). The overall sample volume was 3.00 cm³ in each case. Constant temperature (25.0 ± 0.1 °C) was maintained with an external thermostat and a circulating thermal bath.

Second order reactions of the sulfate ion radical were studied independently in **laser flash photolysis** (hereafter referred to as LFP) experiments. An LKS.60 nanosecond transient absorption spectrometer was applied for the measurements.

The transient species were generated by a Nd:YAG laser and analyzed by a xenon arc lamp in cross-beam (perpendicular) arrangement. Further modules of the LFP setting are a grating monochromator, combined with a photomultiplier and a digital storage oscilloscope.

Transient absorption kinetic curves were registered with the control software of the LFP instrument, Pro-Data LKS and Pro-Data Viewer. Data processing tasks were carried out using Scientist, Excel and Origin programs.

Calculations required for the solution of partial differential equations describing the two-dimensional diffusion in the sulfate ion radical-iodide ion system were carried out using MATLAB R2007a software. Concentrations were calculated by numerical integration using the fourth order Runge-Kutta method (RK4).

III. New scientific results

III.1. On the basis of detailed kinetic studies, a mechanism was proposed and the rate law was determined to interpret the experimental observations in the autoxidation of S(IV) catalyzed by silver(I) ions in the presence of peroxydisulfate ions.

The oxidation kinetics of aqueous S(IV) ($\text{H}_2\text{O}\cdot\text{SO}_2$ and deprotonated forms) by dissolved oxygen (Eq. 1) was studied at low pH values in the presence of AgNO_3 as an added catalyst and $\text{K}_2\text{S}_2\text{O}_8$ as a co-catalyst. The oxidation of S(IV) by $\text{S}_2\text{O}_8^{2-}$ ion drew our attention as a potential subsystem of the autoxidation mechanism of S(IV). The reaction between S(IV) and $\text{S}_2\text{O}_8^{2-}$ ion is very slow at low pH despite the high standard redox potential of the latter. Silver(I) ion was included because it is known to catalyze redox reactions involving $\text{S}_2\text{O}_8^{2-}$ ion, by generating highly reactive intermediates as in (R1).

The reaction rates were determined from the initial phase of the reaction as well as the section preceding the sharp break point on the curves, only apparent in the presence of Ag^+ catalyst. The dependences of the reaction rate on the concentrations of different components and pH imply complex kinetic behavior.

Our data can be interpreted by a chain mechanism (Scheme 1) involving Ag(II) , $\text{SO}_4^{\bullet-}$, $\text{SO}_3^{\bullet-}$ and $\text{SO}_5^{\bullet-}$ radicals as chain carriers. Scheme 1 shows that two initiation steps are operative (R1 and R7) and the major termination step is the recombination of sulfate ion radical into $\text{S}_2\text{O}_8^{2-}$ ions (R9). Ag(III) is an unusually high oxidation state of silver, and is likely to occur in AgO^+ form in aqueous medium. All incorporated steps and species have literature background, including the uncommon oxidation states of silver, Ag(II) and Ag(III) . The presented mechanism exhibits novel features relative to previously described mechanisms in the presence of Ce(III) or iodide ions. Photoinitiation was not required here since Ag(II) and $\text{SO}_4^{\bullet-}$ chain carriers are directly produced in an initiation step. Photochemical interference was avoided in the experimental workset. Furthermore, the disproportionation equilibrium of Ag(II) provides a new path for chain initiation and the reproduction of the catalyst.

Experimental and modelling studies on the reactions of the sulfate ion radical

Based on the suggested mechanism described above, a rather complex rate law can be derived for the overall autoxidation reaction, which is shown in Eq. 2. The rate law is, as expected, zeroth order with respect to the concentration of oxygen and is a complicated function of the concentration of the other components.

$$v = \frac{[\text{S(IV)}](k_{20}[\text{H}^+] + k_{20}'K_a)}{[\text{H}^+] + K_a} \times \quad (2)$$

$$\times \sqrt{\frac{\frac{k_{18}[\text{Ag}^+][\text{S}_2\text{O}_8^{2-}]}{k_{23}}}{1 + \frac{k_{26}[\text{S(IV)}]^2}{k_{23}[\text{Ag}^+]^2} \cdot \left(\frac{k_{20}[\text{H}^+] + k_{20}'K_a}{k_{19}([\text{H}^+] + K_a)}\right)^2 - \frac{k_{24}[\text{Ag}^+]}{[\text{S(IV)}] \frac{k_{25}[\text{H}^+] + k_{25}'K_a}{[\text{H}^+] + K_a} + k_{24}[\text{Ag}^+]}}$$

The rate constants in Eq. (2) are assigned to specific reactions in Scheme 1. Scheme 1 comprises three pH-dependent steps, R3, R5 and R8. The respective rate laws contain the total concentration of S(IV). k_{20}^{obs} , k_{22}^{obs} and k_{25}^{obs} are composite rate constants with similar forms as shown in Eq. 3.

$$k_{20}^{\text{obs}} = \frac{k_{20}[\text{H}^+] + k_{20}'K_a}{[\text{H}^+] + K_a} \quad (3)$$

Here, k_{20} and k_{20}' are the individual rate constants for the different protonated forms of S(IV) and K_a is the acid dissociation constant of hydrated sulfur dioxide.

Non-linear least-squares fitting of Eq. 2 to all the measured data points simultaneously provides an excellent fit, thus corroborating the validity of the proposed kinetic model.

III.2. Second order rate constants for the reactions of $\text{SO}_4^{\bullet-}$ (sulfate ion radical) with numerous small inorganic species and biomolecules were determined by laser flash photolysis.

The sulfate ion radical ($\text{SO}_4^{\bullet-}$) was in the focus of our interest because of its primordial role in the autoxidation mechanisms of S(IV) driven by different catalysts (Ce^{3+} , I^-). $\text{SO}_4^{\bullet-}$ was generated from peroxodisulfate ions by a 266 nm laser pulse, according to Eq. 4, and followed at 450 nm.



Second order rate constants of the reactions of sulfate ion radical were determined with numerous reactants. Pseudo-first order conditions were set wherever possible, using high excess of the given reactant over $\text{SO}_4^{\bullet-}$. The reactions of $\text{SO}_4^{\bullet-}$ with silver(I) ions exhibited pseudo-first order behavior (Figure 2). The value of the second order rate constant is $(6.9 \pm 0.4) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ in neutral solution and $(7.7 \pm 0.5) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ at pH 1.35. In the reaction with Ce^{3+} ions, a rate constant of $(1.18 \pm 0.03) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ was found in strongly acidic medium. The high values of these rate constants confirm the role of $\text{SO}_4^{\bullet-}$ radical as a chain carrier and its ability to activate the catalyst species by rapid oxidation.

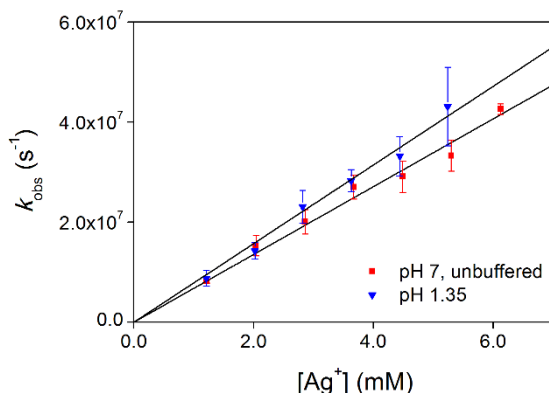


Figure 2. Pseudo-first order rate constant of the reaction between sulfate ion radical and silver(I) ion as a function of silver(I) ion concentration without pH adjustment (■) and in strongly acidic medium (▼). $[\text{K}_2\text{S}_2\text{O}_8] = 0.100 \text{ M}$, $[\text{H}_2\text{SO}_4] = 0.0270 \text{ M}$ (▼), $T = 25 \text{ }^\circ\text{C}$, $V = 3.00 \text{ cm}^3$. Error bars represent the standard deviation of parallel measurements.

Experimental and modelling studies on the reactions of the sulfate ion radical

Iodide ions are known to catalyze the photoinitiated autoxidation of S(IV) efficiently. Kinetic studies in the sulfate ion radical-iodide ion system were carried out at 380 nm, the absorption maximum of I_2^- (iodine molecule anion), which is a strongly absorbing transient species. I_2^- is generated in two consecutive steps, as displayed in Eqs. 5 and 6.



Double exponential kinetic curves were recorded on shorter timescales. Both fitted parameters depend linearly on the concentration of iodide ions (Figure 3). The rate constant with the lower value (line **a**) was assigned to Eq. 5, and the other function (line **b**) corresponds to the reversible process in Eq. 6. The equilibrium constant of reaction 6 could be calculated from the ratio of the slope and intercept of line **b** as $K = (1.74 \pm 0.15) \times 10^3 \text{ M}^{-1}$.

On longer timescales (several milliseconds), the second order decay of I_2^- was observable, conceivably through Eq. 7.

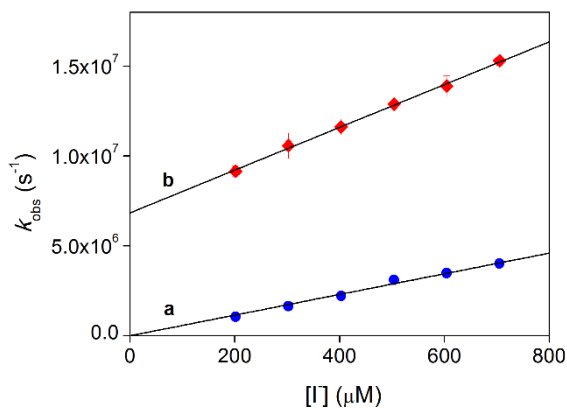


Figure 3. Pseudo-first order rate constants in the reaction between sulfate ion radical and iodide ion on the short time scale. $[K_2S_2O_8] = 0.100 \text{ M}$, $V = 3.00 \text{ cm}^3$, $T = 25 \text{ }^\circ\text{C}$.

Experimental and modelling studies on the reactions of the sulfate ion radical

Kinetic studies on the reactions of $\text{SO}_4^{\bullet-}$ with chloride and bromide ions were undertaken along similar lines. The main difference from the case of iodide ions was that double exponential behavior was no longer detected as chloride and bromide atoms combined more quickly with the respective halide ions. Table 1 gives a summary of the rate constants measured in the sulfate ion radical-halide ion systems. In order to avoid assumptions, the molar absorption coefficients of halide molecule anions are indicated as parameters in the second order rate constants.

Table 1. Rate constants measured during kinetic studies of the reactions of sulfate ion radical with halide ions.

Reaction	k ($\text{M}^{-1} \text{s}^{-1}$)	Conditions
$\text{SO}_4^{\bullet-} + \text{Cl}^-$	$(6.7 \pm 0.2) \times 10^8$	unbuffered
	$(7.5 \pm 0.1) \times 10^8$	pH = 2.03
$\text{SO}_4^{\bullet-} + \text{Br}^-$	$(1.51 \pm 0.02) \times 10^9$	unbuffered
	$(1.59 \pm 0.03) \times 10^9$	pH = 2.03
$\text{SO}_4^{\bullet-} + \text{I}^-$	$(5.7 \pm 0.1) \times 10^9$	unbuffered
$\text{I} + \text{I}^- \rightarrow \text{I}_2^-$	$(1.2 \pm 0.1) \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$	
$\text{I}_2^- \rightarrow \text{I} + \text{I}^-$	$(6.8 \pm 0.3) \times 10^6 \text{ s}^{-1}$	
I_2^- decay	$(4.4 \pm 0.3) \times 10^5 \text{ cm s}^{-1} \times \varepsilon(\text{I}_2^-)$	pH independent
Cl_2^- decay	$(1.40 \pm 0.02) \times 10^5 \text{ cm s}^{-1} \times \varepsilon(\text{Cl}_2^-)$	
Br_2^- decay	$(1.8 \pm 0.1) \times 10^5 \text{ cm s}^{-1} \times \varepsilon(\text{Br}_2^-)$	

Experimental and modelling studies on the reactions of the sulfate ion radical

Exceptional kinetic phenomena in the oxidation processes of tryptophan and derivatives with peroxomonosulfate ions were examined previously in our research group. In relation with these investigations, aromatic amino acids tryptophan (Trp), *N*-tryptophanamide (TrpA) and tyrosine (Tyr) were oxidized by sulfate ion radical. Different amino acid radicals were found to be the products, e.g. Trp^{•+} ($\lambda_{\max} = 580$ nm) as well as TrpN[•] ($\lambda_{\max} = 520$ nm), or tyrosyl radical. The second order rate constants of the reactions of Trp, TrpA and Tyr with sulfate ion radical were measured under pseudo-first order conditions.

The influence of dissolved oxygen and pH was examined. Some of the linear functions that describe the relation between the observed rate constant and the reactant concentration had non-zero vertical intercepts. The determined kinetic parameters are summarized in Table 2.

Table 2. Determined kinetic parameters of the reactions of sulfate ion radical with aromatic amino acid species.

Reactant	Slope ($M^{-1} s^{-1}$)	Intercept (s^{-1})	Conditions
Trp	$(7.4 \pm 0.1) \times 10^9$	—	unbuffered
	$(9.4 \pm 0.5) \times 10^9$	—	pH = 7.21
	$(9.0 \pm 0.3) \times 10^9$	—	pH = 7.21, de-aerated
	$(8.4 \pm 0.8) \times 10^9$	$(1.4 \pm 0.4) \times 10^6$	pH = 7.21, oxygenated
Tyr	$(6.1 \pm 0.1) \times 10^9$	—	acidic, pH not constant
	$(5.1 \pm 0.1) \times 10^9$	—	pH = 2.72
	$(1.4 \pm 0.1) \times 10^9$	$(0.4 \pm 0.3) \times 10^6$	pH = 7.14
TrpA	$(8.8 \pm 0.2) \times 10^9$	$(0.8 \pm 0.2) \times 10^6$	pH = 7.21

III.3. Modelling of the inhomogeneous spatial distribution of the concentration of sulfate ion radical in laser flash photolysis experiments showed that diffusion does not interfere with the determination of second order rate constant with iodide ion under pseudo-first order conditions.

In the reaction between sulfate ion radical and iodide ion, the observed rate constants depend linearly on the concentration of iodide ion (Figure 3). This observation is somewhat contradictory as a sufficiently high excess of iodide ions was in fact not reached *locally* at the site of observation. The potential replacement of iodide ions by diffusion from outside the reaction space was examined by a numerical model. A cylindrical reaction space was considered, defined by the laser beam crossing the cuvette. Initially, the transient species ($\text{SO}_4^{\bullet-}$) were located inside this cylinder. Their concentration was maximal at the front face of the cuvette and decreased along the laser beam axis. The absorbance was measured perpendicularly to the laser pulse just as in the experiments. Iodide ions were distributed homogeneously. Mass transport was allowed between the reaction space and an external cylinder defined in the model.

The random walk model of diffusion was applied to simplify the solution of the describing partial differential equation (PDE) system 8. Here, \mathbf{c} is the vector of concentrations, \mathbf{D} is the matrix of diffusion constants, \mathbf{R} is an operator containing the ongoing reactions and Δ is the Laplacian.

$$\frac{\partial \mathbf{c}}{\partial t} = \mathbf{D}\Delta \mathbf{c} + \mathbf{R}(\mathbf{c}) \quad (8)$$

The Laplacian operator in Eq. 8 takes the form of Eq. 9 in cylindrical coordinates (x, r, ϕ) .

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} \quad (9)$$

The angular term in Eq. 9 could be omitted in our case, because the reaction space was cylindrically symmetric, as a consequence of the uniform energy distribution of the laser pulse. This facilitated the solution of Eq. 8 significantly. The partial derivative with regards to x and r were approximated by the finite difference method, using central differences. Diffusion in axis (x) and radius (r) directions could be described with matrix multiplication.

Experimental and modelling studies on the reactions of the sulfate ion radical

The reaction space was divided into unit volumes shaped like cylinder rings. Matter exchange took place between the unit volumes proportionally to the common surface area and the concentration gradient between two neighboring cells according to Fick's first law.

To test the validity of the algorithm, only the diffusive motion of the species was followed first, without the reaction. It was found that the law of mass conservation is fulfilled, $\text{SO}_4^{\bullet-}$ radicals reached homogeneous distribution in the reaction space and the concentration of iodide ion remained constant.

The model was then expanded with the second order reaction of $\text{SO}_4^{\bullet-}$ and I^- . The total concentration of sulfate ion radicals rapidly decreased to 0 in this case and a homogeneous distribution was not reached in the reaction space before their concentration dropped to 1% of its original value.

Using the experimentally measured rate constant as an input parameter ($5.7 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$), we simulated the kinetic traces and determined the values of pseudo-first order rate constants (k_{obs}) from these traces. The calculated kinetic curves gave a very good fit to an exponential function if iodide ion was in at least 2.5-fold excess over sulfate ion radical ($4 \times 10^{-4} : 1 \times 10^{-3} \text{ M}$). Figure 4 shows the close similarity between the calculated and the experimental values, meaning that diffusion does not influence the determination of the rate constant within the time frame of the reaction.

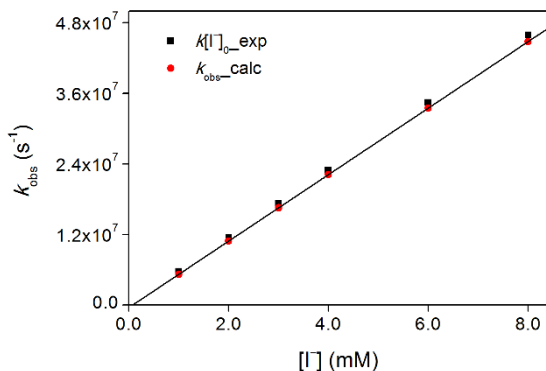


Figure 4. Comparison of the calculated and experimental pseudo-first order rate constants as a function of initial iodide ion concentrations ($c_{\text{B}0}$ in the model).

IV. Possible applications of the results

Autoxidation studies of sulfur(IV) have been an interest of inorganic chemistry in the last few decades, mostly because of its role in acid rain formation. Deeper understanding of transition metal catalysis in such atmospheric aqueous processes can promote the development of 'green' oxidation catalysts and catalytic procedures. They can also assist the targeted application of free radicals to remove organic and inorganic contaminants from natural water supplies. Wastewater treatment using $\text{SO}_4^{\bullet-}$ as oxidant is already in active use (Advanced Oxidation Processes, AOPs).

The one-electron oxidation of aromatic amino acid residues within oligopeptides and proteins is a rich research area. In some known cases, free radicals within enzymes contribute to the catalytic activity. Such an example is ribonucleotide reductase, in which a tyrosine radical in the close vicinity of the active site plays essential role in the function of the enzyme. The number of possibilities for the location of the lack of electron and the abundance of redox active residues (Cys, Met, Tyr, Trp) render protein radical studies overly complicated. Detailed understanding requires simultaneous application of fast kinetic methods, such as flash photolysis or pulse radiolysis, EPR, spin trapping and quenching methods as well as theoretical approaches. The one-electron oxidation of biomolecules is still overshadowed by two-electron processes, radical procedures are often significantly harder to disclose. Common efforts of chemists, biologists and computation experts are required to fully understand such processes.

Our numerical calculations aiming to describe spatial inhomogeneities in laser flash photolysis experiments draw attention to the possible effect of insufficient mixing in fast kinetic experiments. The arguments presented here also raise awareness to the fact that inhomogeneous distribution of reactants can influence the results of standard kinetic data processing, especially where pseudo-first order conditions are not met in the system and second or even higher order kinetics is operative.

V. Publications

V.1. Papers related to the thesis

4. Éva Dóka, Gábor Lente

Modelling studies of inhomogeneity effects during laser-flash photolysis experiments: a reaction-diffusion approach

manuscript in preparation

3. Éva Dóka, Gábor Lente, István Fábíán

The reactivity of the sulfate ion radical

manuscript in preparation

2. Éva Dóka, Gábor Lente, István Fábíán

Kinetics of the autoxidation of sulfur(IV) co-catalyzed by peroxodisulfate and silver(I) ions

Dalton Transactions, **2014**, 43, 9596-9603.

IF: 4.197

1. József Kalmár, Éva Dóka, Gábor Lente, István Fábíán

Aqueous photochemical reactions of chloride, bromide, and iodide ions in a diode-array spectrophotometer. Autoinhibition in the photolysis of iodide ions

Dalton Transactions, **2014**, 43, 4862-4870.

IF: 4.197

V.2. Lectures related to the thesis

6. Éva Dóka, Lente Gábor, Fábíán István

Térbeli inhomogenitás modellezése villanófény-fotolízis kísérletekben
Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences

26 May 2014, Siófok, Hungary

5. István Fábíán, Éva Dóka, Gábor Lente

Kinetic Studies on the Reactions of the Sulfate Ion Radical

Second EuCheMS Inorganic Chemistry Conference

7-11 July 2013, Jerusalem, Israel

Experimental and modelling studies on the reactions of the sulfate ion radical

4. Éva Dóka, Gábor Lente, István Fábán

A szulfátiongyök reakcióinak tanulmányozása lézeres villanófény-fotolízissel
Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences

26 October 2012, Gyöngyöstarján, Hungary

3. Éva Dóka, Gábor Lente, István Fábán

Laser Flash Photolysis Studies on the Reactions of the Sulfate Ion Radical
46th Colloquium of Coordination Chemistry

21 May 2012, Mátrafüred, Hungary

2. Éva Dóka, Gábor Lente, István Fábán

A kén(IV) autooxidációja ezüst(I)- és peroxodiszulfát ionok jelenlétében
Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences

24 April 2009, Balatonalmádi, Hungary

1. Dóka Éva

A kén(IV) autooxidációja ezüst(I)- és peroxodiszulfát-ionok jelenlétében
31th Scientific Students' Association Conference

6 April 2009, Debrecen, Hungary

V.3. Posters related to the thesis

5. Éva Dóka, Gábor Lente, István Fábán

Modeling spatial inhomogeneity in laser flash photolysis experiments
European Colloquium on Inorganic Reaction Mechanisms

17-20 June 2014, Debrecen, Hungary

4. Éva Dóka, Gábor Lente, István Fábán

Laser flash photolysis studies on the reactions of the sulfate ion radical
International Conference on Chemical Kinetics

8-13 July 2013, Seville, Spain

3. Éva Dóka, Gábor Lente, István Fábán

Laser flash photolysis studies on the reactions of the sulfate ion radical
Debrecen Colloquium on Inorganic Reaction Mechanisms

11-15 June 2013, Debrecen, Hungary

Experimental and modelling studies on the reactions of the sulfate ion radical

2. Éva Dóka, Gábor Lente, István Fábián

Laser flash photolysis studies on the reactions of the sulfate ion radical

Gordon Research Conferences, Inorganic Reaction Mechanisms

3-8 March 2013, Galveston, Texas, USA

1. Éva Dóka, Gábor Lente, István Fábián

The autoxidation of sulfur(IV) in the presence of silver(I) and peroxodisulfate ions

Inorganic Reaction Mechanism Group Meeting

7-10 January 2010, Kloster Banz, Germany

V.4. Papers not related to the thesis

5. Éva Dóka, Irina Pader, Adrienn Bíró, Katarina Johansson, Qing Cheng, Krisztina Ballagó, Justin R. Prigge, Daniel Pastor-Flores, Tobias P. Dick, Edward E. Schmidt, Elias S. J. Arnér, Péter Nagy

Novel persulfide detection method reveals protein persulfide- and polysulfide-reducing functions of thioredoxin and glutathione systems

Science Advances, **2016**, 2, e1500968.

IF: N/A

4. Anita Vasas, Éva Dóka, István Fábián, Péter Nagy

Kinetic and thermodynamic studies on the disulfide-bond reducing potential of hydrogen sulfide

Nitric Oxide, **2014**, 46, 93-101.

IF: 3.521

3. David Peralta, Agnieszka K. Bronowska, Bruce Morgan, Éva Dóka, Koen van Laer, Péter Nagy, Frauke Gräter, Tobias P. Dick

A proton relay enhances H₂O₂ sensitivity of GAPDH to facilitate metabolic adaptation

Nature Chemical Biology, **2015**, 11, 156-63.

IF: 12.996

2. Éva Dóka, Gábor Lente

Stochastic mapping of the Michaelis-Menten mechanism

Journal of Chemical Physics, **2012**, 136, 054111.

IF: 3.164

Experimental and modelling studies on the reactions of the sulfate ion radical

1. Éva Dóka, Gábor Lente

Mechanism-Based Chemical Understanding of Chiral Symmetry Breaking in the Soai Reaction. A Combined Probabilistic and Deterministic Description of Chemical Reactions

Journal of the American Chemical Society, **2011**, *133*, 17878-17881. IF: 9.907

V.5. Lectures not related to the thesis

7. Éva Dóka, Irina Pader, Adrienn Bíró, Katarina Johansson, Qing Cheng, Krisztina Ballagó, Justin R. Prigge, Daniel Pastor-Flores, Tobias P. Dick, Ed Schmidt, Elias S. J. Arnér, Péter Nagy

Fehérje perszulfid poszttranszlációs módosulatok képződésének és redukációjának vizsgálatai

Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences

6 November 2015, Mátrafüred, Hungary

6. Éva Dóka, David Peralta, Agnieszka K. Bronowska, Bruce Morgan, Koen Van Laer, Frauke Gräter, Tobias P. Dick, Péter Nagy

A glicerinaldehid-3-foszfát-dehidrogenáz enzim redox regulációjának molekuláris mechanizmusa

Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences

27 March 2015, Debrecen, Hungary

5. Gábor Lente, Éva Dóka

Stochastic Kinetic Modeling of the Soai Reaction

4th EuCheMS Chemistry Congress

26 August 2012, Prague, Czech Republic

4. Gábor Lente, Éva Dóka

Stochastic Kinetic Modeling of the Soai Reaction

46th Colloquium of Coordination Chemistry

21 May 2012, Mátrafüred, Hungary

Experimental and modelling studies on the reactions of the sulfate ion radical

3. Dóka Éva

A Soai-reakció sztochasztikus kinetikai elemzése

30th Scientific Students' Association Conference

29 April 2011, Pécs, Hungary

2. Gábor Lente, Éva Dóka

Monte Carlo interpretation of the distribution of enantiomers formed in the Soai reaction

2nd International Symposium on the Soai Reaction and Related Topic

11-13 September 2010, Felsőmocsolád, Hungary

1. Éva Dóka, Gábor Lente

A Soai-reakció értelmezése Monte Carlo módszerrel (Monte Carlo interpretation of the Soai reaction)

Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences

29 April 2010, Balatonalmádi, Hungary

V.6. Posters not related to the thesis

2. Éva Dóka, Adrienn Bíró, Zoltán Pálinkás, Ming Xian, Tobias P. Dick, Péter Nagy

A novel method for protein persulfide measurement presented on the example of human serum albumin sulphydration in blood plasma

ESF-EMBO Symposium – Thiol based redox switches in life sciences

12-17 September 2015, San Feliu de Guixols, Spain

1. Anita Vasas, Éva Dóka, István Fábián, Péter Nagy

Kinetic and thermodynamic studies on the disulfide-bond reducing potential of hydrogen sulfide

3rd European Conference on the Biology of Hydrogen Sulfide

3-6 May 2015, Athens, Greece



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Candidate: Éva Dóka
Neptun ID: LZPX6E
Doctoral School: Doctoral School of Chemistry
MTMT ID: 10032840

List of publications related to the dissertation

Foreign language scientific article(s) in international journal(s) (2)

1. Kalmár, J., **Dóka, É.**, Lente, G., Fábíán, I.: Aqueous photochemical reactions of chloride, bromide, and iodide ions in a diode-array spectrophotometer. Autoinhibition in the photolysis of iodide ions.
Dalton Trans. 43 (12), 4862-4870, 2014. ISSN: 1477-9226.
DOI: <http://dx.doi.org/10.1039/c3dt53255k>
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Experimental and modelling studies on the reactions of the sulfate ion radical



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IF: 9.907

Total IF of journals (all publications): 37,982

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The Candidate's publication data submitted to the IDEa Tudóstér have been validated by DEENK on the basis of Web of Science, Scopus and Journal Citation Report (Impact Factor) databases.

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