

Publication List

Original Research Papers:

36. Gábor Lente

Thermodynamic unfeasibility of recycling in chiral autocatalytic kinetic models
Reaction Kinetics and Catalysis Letters, **2008**, *in press*.

35. Victor Polshin, Delia-Laura Popescu, Andreas Fischer, Arani Chanda, David C. Horner, Evan S. Beach, Jennifer Henry, Yong-Li Qian, Colin P. Horwitz, Gábor Lente, István Fábián, Eckard Münck, Emile L. Bominaar, Alexander D. Ryabov, Terrence J. Collins

Attaining Control by Design over the Hydrolytic Stability of Fe-TAML Oxidation Catalysts

Journal of the American Chemical Society, **2008**, *130*, 4497-4506.

34. Gábor Lente

The effect of parity violation on kinetic models of enantioselective autocatalysis
Physical Chemistry Chemical Physics, **2007**, *9*, 6134-6141.

33. Gábor Lente, István Fábián

Kinetics and Mechanism of the Oxidation of Water Soluble Porphyrin Fe^{III}TPPS with Hydrogen Peroxide and Peroxomonosulfate Ion

Dalton Transactions, **2007**, 4268-4275.

32. Gábor Lente, István Fábián, György Bazsa

What is and what isn't a clock reaction?

New Journal of Chemistry, **2007**, *31*, 1707-1707.

31. Mónika Galajda, Gábor Lente, István Fábián

Photochemically induced autocatalysis in the chlorate ion-iodine system

Journal of the American Chemical Society, **2007**, *129*, 7738-7739.

30. Ildikó Kerezi, Gábor Lente, István Fábián

Kinetics and Mechanism of the Photoinitiated Autoxidation of Sulfur(IV) in the Presence of Iodide Ion

Inorganic Chemistry, **2007**, *46*, 4230-4238.

29. Gábor Lente

Stochastic analysis of the parity violating energy differences between enantiomers and its implications for the origin of biological chirality

Journal of Physical Chemistry A, **2006**, *110*, 12711-12713.

28. Ildikó Kerezi, Gábor Lente, István Fábián

Kinetics of the light-driven aqueous autoxidation of sulfur(IV) in the absence and presence of iron(II)

Dalton Transactions, **2006**, 955-960.

27. Gábor Lente

Stochastic kinetic models of chiral autocatalysis: a general tool for the quantitative interpretation of total asymmetric synthesis

Journal of Physical Chemistry A, **2005**, *109*, 11058-11063.

26. Gábor Lente, István Fábián, Anthony J. Poë
A common misconception about the Eyring equation

New Journal of Chemistry, **2005**, *29*, 759-760.

25. Ildikó Kerecsi, Gábor Lente, István Fábián
Highly Efficient Photoinitiation in the Cerium(III)-Catalyzed Aqueous Autoxidation of Sulfur(IV). An Example of Comprehensive Evaluation of Photoinduced Chain Reactions

Journal of the American Chemical Society, **2005**, *127*, 4785-4793.

24. Katalin Ósz, Gábor Lente, Csilla Kállay
New protonation microequilibrium treatment in the case of some amino acid and peptide derivatives containing bis(imidazolyl)methyl group

Journal of Physical Chemistry B, **2005**, *109*, 1039-1047.

23. Gábor Lente, James H. Espenson
Oxidation of 2,4,6-Trichlorophenol by Hydrogen Peroxide. Comparison of Different Iron-Based Catalysts

Green Chemistry, **2005**, *7*, 28-34.

22. Gábor Lente
Homogeneous Chiral Autocatalysis: a Simple, Purely Stochastic Kinetic Model

Journal of Physical Chemistry A, **2004**, *108*, 9475-9478.

21. Gábor Lente, James H. Espenson
A Kinetic Study of the Early Steps in the Oxidation of Chlorophenols by Hydrogen Peroxide Catalyzed by a Water-Soluble Iron(III) Porphyrin

New Journal of Chemistry, **2004**, *28*, 847-852.

20. Gábor Lente, István Fábián
Effect of Dissolved Oxygen on the Disproportionation and Oxidation of the Dithionate Ion. Extremely Unusual Kinetic Traces

Inorganic Chemistry, **2004**, *43*, 4019-4025.

19. Gábor Lente, James H. Espenson
Unusual Kinetic Role of a Water-Soluble Iron(III) Porphyrin Catalyst in the Oxidation of 2,4,6-Trichlorophenol by Hydrogen Peroxide

International Journal of Chemical Kinetics, **2004**, *36*, 449-455.

18. Gábor Lente, James H. Espenson
Photoreduction of 2,6-Dichloroquinone in Aqueous Solution. Use of a Diode Array Spectrophotometer Concurrently to Drive and Detect a Photochemical Reaction

Journal of Photochemistry and Photobiology A: Chemistry, **2004**, *163*, 249-258.

17. József Emri, Gábor Lente

Use of an electron equivalent relationship between bond length and bond order to study chemical bonding. Part II. A study of bond orders, bond lengths and aromaticity in polycyclic aromatic hydrocarbons

Journal of Molecular Structure (THEOCHEM), **2004**, 671, 211-219.

16. Ildikó Kerecsi, Gábor Lente, István Fábán

Complex Formation Reaction of the Iron(III) Hydroxo Dimer with Periodate Ion

Dalton Transactions, **2004**, 342-346.

15. Gábor Lente, James H. Espenson

Photoaccelerated oxidation of chlorinated phenols

Chemical Communications, **2003**, 1162-1163.

14. James H. Espenson, Xiaopeng Shan, Ying Wang, Ruili Huang, David W. Lahti, JaNeille Dixon, Gábor Lente, Arkady Ellern, Ilia A. Guzei

Synthesis and Characterization of Dimetallic Oxorhenium(V) and Dioxorhenium(VII) Compounds, and a Study of Stoichiometric and Catalytic Reactions

Inorganic Chemistry, **2002**, 41, 2583-2591.

13. Ying Wang, Gábor Lente, James H. Espenson

Oxorhenium(V) Dithiolates Catalyze the Oxidation by tert-Butyl Hydroperoxide of Sulfoxides and Sulfides, including 4,6-Dimethyldibenzothiophene

Inorganic Chemistry, **2002**, 41, 1272-1280.

12. Gábor Lente, István Fábán

Ligand Substitution Kinetics of the Iron(III) Hydroxo Dimer with Simple Inorganic Ligands

Inorganic Chemistry, **2002**, 41, 1306-1314.

11. Gábor Lente, István Fábán

Kinetics and mechanism of the oxidation of sulfur(IV) by iron(III) at metal ion excess

J. Chem. Soc., Dalton Trans., **2002**, 778-784.

10. Gábor Lente, István Fábán

A Simple Test to Confirm the Ligand Substitution Reactions of the Hydrolytic Iron(III) Dimer

Reaction Kinetics and Catalysis Letters, **2001**, 73, 117-125.

9. Gábor Lente, James H. Espenson

Kinetics and Mechanism of Oxygen Transfer to Methyloxo(dithiolato)rhenium(V) Complexes

Inorganic Chemistry, **2000**, 39, 4809-4814.

8. Gábor Lente, Xiao-Peng Shan, Ilia A. Guzei, James H. Espenson

Syntheses and Structures of Rhenium(IV) and Rhenium(V) Complexes with Ethanedithiolato Ligands

Inorganic Chemistry, **2000**, 39, 3572-3576.

7. Gábor Lente, M. Elizabeth A. Magalhães, István Fábián
Kinetics and Mechanism of Complex Formation Reactions in the Iron(III)-Phosphate Ion System at Large Iron(III) Excess. The Formation of a Tetranuclear Complex
Inorganic Chemistry, **2000**, *39*, 1950-1954.
6. Gábor Lente, Ilia A. Guzei, James H. Espenson
Kinetics and Mechanism of the Monomerization of a Re(V) Dithiolato Dimer with Monodentate Ligands. Electronic and Steric Effects
Inorganic Chemistry, **2000**, *39*, 1311-1319.
5. Gábor Lente, Josemon Jacob, Ilia A. Guzei, James H. Espenson
Kinetics and Crystallographic Studies of the Ligand Monomerization of a Dithiolato(methyl)(oxo)rhenium(V) Dimer
Inorganic Reaction Mechanisms, **2000**, *2*, 169-177.
4. Josemon Jacob, Gábor Lente, Ilia A. Guzei, James H. Espenson
Monomerization of a Rhenium(V) Dimer by Ligation
Inorganic Chemistry, **1999**, *38*, 3762-3763.
3. Gábor Lente, István Fábián
A New Reaction Path in the Dissociation of the $\text{Fe}_2(\mu\text{-OH})_2(\text{H}_2\text{O})_8^{4+}$ Complex
Inorganic Chemistry, **1999**, *38*, 603-605.
2. Gábor Lente, A. Mark Dobbing, David T. Richens
Kinetic Studies of Water Exchange and Substitution by NCS^- on the Sulphur-capped Triangular Ion $[\text{Mo}_3(\mu_3\text{-S})(\mu\text{-O})_3(\text{OH}_2)_9]^{4+}$
Inorganic Reaction Mechanisms, **1998**, *1*, 3-16.
1. Gábor Lente, István Fábián
The Early Phase of the Iron(III) Sulfite Ion Reaction. The Formation of a Novel Iron(III)-Sulfite Complex
Inorganic Chemistry, **1998**, *37*, 4204-4209.

Letters and Comments

4. Gábor Lente
EURYI: present procedure risks conflicts of interest
Nature, **2005**, *437*, 192. (IF 2004: 29.273)
3. Gábor Lente
Time to stop blaming communism in Hungary
Nature, **2004**, *428*, 17. (IF 2004: 32.182)

2. Gábor Lente

Don't Be Tricked by Your Integrated Rate Plot: Pitfalls of Using Integrated Rate Plots

Journal of Chemical Education, **2004**, *81*, 32. (IF 2004: 0.507)

1. Gábor Lente

The New Hungarian Science Programs

Science, **2002**, *295*, 625. (IF 2002: 26.682)

InternetWatch

Chemistry animations and movies on the World Wide Web

Chemistry Magazine, (ACS) Winter **2003**, 6.

Chemistry Goes to the Movies

Science, **2002**, 296, 1371.

Popular Science Magazines

Ózon – egyszerre kevés és sok

Természet Világa **2005**, 136, 416.

Kadmiumtartalmú fehérjét találtak

Természet Világa **2005**, 136, 416.

Lente Gábor

Elemnévadás az uránon túl

Középiskolai Kémiai Lapok, **2007**, 34, 345-351.

Lente Gábor

Jég-kilenc a Macskabölcsőben

Középiskolai Kémiai Lapok, **2008**, 35, 1-9.

Books and Book Chapters

2. Z. Fekete, S. Igaz, D. Komáromy, A. Kotschy, G. Kóczán, G. Lente, G. Magyarfalvi, A. Nagy, I. Pálinkó, A. Stirling, L. Túri, J. Zádor: *'Preparatory problems for the 40th International Chemistry Olympiad'*, Ed: G. Magyarfalvi, 2008, 40th International Chemistry Olympiad, Budapest, ISBN 978-963-463-965-7

1. Lente, G. *'Oxidation of Halogenated and Polycyclic Aromatic Hydrocarbons using Rhenium-Based Catalysts'* in *'My Fulbright Experience'* Dietz, K. (ed.), Hungarian-American Commission for Educational Exchange, Budapest, 2006, pp. 77-90, ISBN: 963 216 798 8.

Invited Seminars at Academic Institutions:

13. Gábor Lente

Vas(III)-komplexek katalitikus szerepe klórfenolok teljes kémiai lebontásában (Iron(III) complexes as catalysts in the total chemical destruction of chlorophenols)
University of Szeged, *Inorganic Chemistry Seminar*, November 9, 2006, Szeged, Hungary.

12. Gábor Lente

Sztocasztikus kinetikai hatások a királis autokatalízisben (Stochastic kinetic effects in chiral autocatalysis)
University of Szeged, *Physical Chemistry Seminar*, April 25, 2006, Szeged, Hungary.

11. Gábor Lente

Iron complexes as catalysts in the total chemical destruction of chlorophenols
Eötvös Loránd University, *Inorganic Chemistry Seminar*, October 13, 2005, Budapest, Hungary.

10. Gábor Lente

Diódasoros spektrofotométerek fényének hatása kémiai reakciókra (Influence of the light of diode array spectrophotometers on chemical reactions)
University of Debrecen, *Physical Chemistry Seminar*, September 28, 2005, Debrecen, Hungary.

9. Gábor Lente

Spektrofotométerek fényének kémiai szerepe kinonok oldatreakcióiban és a kén-dioxid vizes közegű autooxidációjában (Influence of the light of spectrophotometers on some solution reactions of quinones and the aqueous autoxidation of sulfur dioxide)
Hungarian Academy of Sciences, March 11, 2005, Budapest, Hungary.

8. Gábor Lente

Catastrophic Cyanide Pollution in a Central European River System
Iowa State University, *ACS (American Chemical Society) Seminar*, April 3, 2003, Ames, IA, USA.

7. Gábor Lente

Reactions of the Dithionate Ion: Disproportionation and Oxidation
New Mexico State University, *Inorganic Chemistry Seminar*, March 13, 2003, Las Cruces, NM, USA.

6. Gábor Lente

Catastrophic Cyanide Pollution in a Central European River System
New Mexico State University, *MARC (Minority Access to Research Careers) Seminar*, March 12, 2003, Las Cruces, NM, USA.

5. Gábor Lente

Catastrophic Cyanide Pollution in a Central European River System
University of California at Los Angeles, *Inorganic Chemistry Seminar*, February 21, 2003, Los Angeles, CA, USA.

4. Gábor Lente

Reactions of the Iron(III) Hydroxo Dimer

University of Minnesota at Minneapolis, *Invited Seminar*, January 17, 2003, Minneapolis, MN, USA.

3. Gábor Lente

Catastrophic Cyanide Pollution in a Central European River System

Iowa State University, *Inorganic Chemistry Seminar*, September 18, 2002, Ames, IA, USA.

2. Gábor Lente

Reactivity of new methyl(oxo)rhenium(V) complexes

Miami University, *Chemistry Seminar*, November 18, 1999, Oxford, OH, USA.

1. Gábor Lente

Reactivity of new methyl(oxo)rhenium(V) complexes

Iowa State University, *Inorganic Chemistry Seminar*, September 15, 1999, Ames, IA, USA.

Other presentations

6. Gábor Lente (lecture in Hungarian)

Drágakövek és nemesfémek (Precious stones and metals)

Great Forest Tales about Chemistry Seminar Series (Nagyerdei Mesék a Kémiáról), November 19, 2007, Debrecen, Hungary

5. Gábor Lente (lecture in Hungarian)

'Mai molekulatudomány mindenkinek avagy Hogyan vegyünk rá

jogászhallgatókat a kémiatanulásra? (Modern Molecular Science for Everyone or How to convince law majors to study chemistry)

University of Debrecen, *Physical Chemistry Seminar*, October 3, 2007, Debrecen, Hungary.

4. Gábor Lente (lecture in Hungarian)

'Mai molekulatudomány mindenkinek avagy Hogyan vegyünk rá

jogászhallgatókat a kémiatanulásra? (Modern Molecular Science for Everyone or How to convince law majors to study chemistry)

Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, April 26-27, 2007, Balatonalmádi, Hungary.

3. Gábor Lente (lecture in Hungarian)

'Impact factor, preprint, open access' - kulcsszavak a tudományos publikáció

jövőjéről folytatott vitában ('Impact factor, preprint, open access - buzzwords in the debate about the future of scientific publication)

Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, April 29-30, 2004, Balatonalmádi, Hungary.

2. Gábor Lente

The Fulbright Experience: a Year at Iowa State, Ames

Meeting of Fulbright Alumni, January 21, 2004, Budapest, Hungary.

1. Gábor Lente

Lajos Kossuth: A Personal View

Iowa State University, Invited Presentation, September 19, 2002, Ames, IA, USA.

Conferences:

62. Gábor Bellér, Gábor Lente, István Fábián (lecture in Hungarian)

Redukció oxidálószer hatására? A ferriin egy meglepő reakciója (Reduction upon the addition of an oxidant? A surprising reaction of ferriin)

43rd Colloquium on Coordination Chemistry, May 28-30, 2008, Siófok, Hungary.

61. Gábor Lente, Tamás Ditrói (lecture in Hungarian)

Királis autokatalízis és kölcsönös antagonizmus: a Frank-modell sztochasztikus elemzése (Chiral autocatalysis and mutual antagonism: a stochastic analysis of the Frank-model)

Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, April 17-18, 2008, Balatonalmádi, Hungary.

60. Mónika Galajda, Gábor Lente, István Fábián (lecture)

Photochemically confused exotic phenomena in the chlorate ion – iodine system

37th Inorganic Reaction Mechanisms Group Meeting, January 9-12, 2008, Barcelona, Spain.

59. Gábor Lente, Dávid Bajusz, Marcell Takács, Lilla Veres, István Fábián (poster)

Reactions of the peroxomonosulfate ion with halide ions

37th Inorganic Reaction Mechanisms Group Meeting, January 9-12, 2008, Barcelona, Spain.

58. Gábor Lente (lecture in Hungarian)

Vízoldható vas(III)-porfirin komplex katalitikus hatása klórfenolok kémiai lebontásában (Catalytic role of a water-soluble iron(III) porphyrin complex in the chemical destruction of chlorophenols)

Meeting of the Coordination Chemistry Working Group of the Hungarian Academy of Sciences, December 10, 2007, Budapest, Hungary.

57. Gábor Lente, Dávid Bajusz, Marcell Takács, Lilla Veres, István Fábián (lecture in Hungarian)

A peroxomonoszulfát-ion reakciói halogenidionokkal (Reactions of the peroxomonosulfate ion with halide ions)

Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, October 25-26, 2007, Gyöngyöstarján, Hungary.

56. Gábor Bellér, Gábor Lente, István Fábián (lecture in Hungarian)

A peroxomonoszulfát-ion reakciója ferroinnal (Reaction of peroxomonosulfate ion

with ferroun)

42nd Colloquium on Coordination Chemistry, May 23-25, 2007, Mátrafüred, Hungary.

55. Gábor Lente (lecture in Hungarian)

A paritásértés-energia hatása a királis autokatalízisben (Parity violation energy in chiral autocatalysis)

Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, April 26-27, 2007, Balatonalmádi, Hungary.

54. Mónika Galajda, Gábor Lente, István Fábán (lecture in Hungarian)

Fotokémiai hatások a klorátion-jód reakcióban (Photochemical effects in the chlorate ion-iodine reaction)

Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, April 26-27, 2007, Balatonalmádi, Hungary.

53. Gábor Lente, Gábor Bellér, József Kalmár, Zsuzsa Baranyai, Alíz Kun, Ildikó Kék, István Fábán (poster and lecture)

Reactions of the peroxomonosulfate ion with simple inorganic reducing agents

Gordon Research Conference, Inorganic Reaction Mechanisms, February 18 - 23, 2007, Ventura, CA, USA.

52. Gábor Lente, Gábor Bellér, József Kalmár, Zsuzsa Baranyai, Alíz Kun, Ildikó Kék, István Fábán (lecture in Hungarian)

A peroxomonosulfát-ion reakciói egyszerű szervetlen redukálószerekkel

(Reactions of the peroxomonosulfate ion with simple inorganic reducing agents)

Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, November 2-3, 2006, Gyöngyöstarján, Hungary.

51. Gábor Lente, József Emri (poster)

Experimental bond order for metal-metal bonding

1st European Chemistry Congress, August 27-31, 2006, Budapest, Hungary

50. Gábor Lente, Szabina Deák, István Fábán (lecture in Hungarian)

Fe^{III}(TAML) komplex reakciója hidrogén-peroxiddal (Reaction of Fe^{III}(TAML) with hydrogen peroxide)

41st Colloquium on Coordination Chemistry, May 31-June 2, 2006, Mátrafüred, Hungary.

49. József Emri, Gábor Lente (lecture in Hungarian)

Létezik-e ötös illetve hatos fém-fém kötés? (Are there examples of quintuple or sextuple metal-metal bonds?)

41st Colloquium on Coordination Chemistry, May 31-June 2, 2006, Mátrafüred, Hungary.

48. Ildikó Kerecsi, Gábor Lente, István Fábán (lecture in Hungarian)

Fény derült a kén(IV) autooxidációjára (Sulfur(IV) autoxidation enlightened)

41st Colloquium on Coordination Chemistry, May 31-June 2, 2006, Mátrafüred, Hungary.

47. Gábor Lente (lecture in Hungarian)

Általános sztochasztikus kinetikai modellek abszolút aszimmetrikus reakciók értelmezésére (General stochastic kinetic models for the interpretation of total

asymmetric synthesis)

Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, April 27-28, 2006, Balatonalmádi, Hungary.

46. Ildikó Kerecsi, Gábor Lente, István Fábián (lecture)

Sulfur(IV) autoxidation enlightened

35th Inorganic Reaction Mechanisms Group Annual Meeting, January 4-7, 2006, Krakow, Poland.

45. Gábor Lente, István Fábián (lecture)

Kinetics of the reaction between water-soluble iron(III) porphyrin Fe(TPPS) and hydrogen peroxide

35th Inorganic Reaction Mechanisms Group Annual Meeting, January 4-7, 2006, Krakow, Poland.

44. József Kalmár, Gábor Lente, István Fábián (lecture in Hungarian)

Halogenidionok vizes oldatbeli fotolízise (Photolysis of halide ions in aqueous solution)

Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, October 20-21, 2005, Gyöngyöstarján, Hungary.

43. Ildikó Kerecsi, Gábor Lente, István Fábián (poster)

Photoinitiated catalytic aqueous autoxidation of sulfur(IV)

International Conference on Solution Chemistry, August 20 - 25, 2005, Portoroz, Slovenia

42. Gábor Lente, István Fábián (lecture in Hungarian)

Fe^{III}(TPPS) vízoldható porfirin sztöchiometrikus és katalitikus reakciói hidrogén-peroxiddal és peroxomonoszulfáttal (Stoichiometric and catalytic reactions of the water-soluble porphyrin Fe^{III}(TPPS) with hydrogen peroxide and peroxomonosulfate ion)

40th Colloquium on Coordination Chemistry, May 18-20, 2005, Dobogókő, Hungary.

41. Ildikó Kerecsi, Gábor Lente, István Fábián (lecture in Hungarian)

A fény hatása a kén-dioxid katalitikus autooxidációjára (Effect of light on the catalytic autoxidation of sulfur dioxide)

Annual Conference for Graduate Students, May 5-8, 2005, Debrecen, Hungary.

40. Ildikó Kerecsi, Gábor Lente, István Fábián (lecture in Hungarian)

Fotokémiai reakciók a vas(II)-szulfition-oxigén rendszerben (Photochemical reactions in the iron(II)-sulfite ion-oxygen system)

Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, April 28-29, 2005, Balatonalmádi, Hungary.

39. István Fábián, Gábor Lente (lecture in Hungarian)

Tévhit, hitek és tények az oldatfázisú reakciók aktiválási paramétereivel kapcsolatban (Activation parameters in solution kinetics: use, misuse, and abuse)

Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, April 28-29, 2005, Balatonalmádi, Hungary.

38. Gábor Lente, István Fábián (lecture in Hungarian)
Fe(TPPS) vízoldható porfirin reakciója hidrogén-peroxiddal és peroxomonosulfátiónnal (Oxidation of the water-soluble porphyrin Fe(TPPS) with hydrogen peroxide and peroxomonosulfate ion)
Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, April 28-29, 2005, Balatonalmádi, Hungary.
37. Gábor Lente, Ildikó Kerecsi, István Fábián (poster)
Photoinitiated aqueous autoxidation of sulfite ion: comparison of cerium(III) and iodide catalysis
Gordon Research Conference, Inorganic Reaction Mechanisms, February 13 - 18, 2005, Ventura, CA, USA.
36. Ildikó Kerecsi, Gábor Lente, István Fábián (poster)
Photoinitiated aqueous autoxidation of sulfur(IV): comparison of cerium(III) and iodide catalysis
34th Inorganic Reaction Mechanisms Group Annual Meeting, January 5-7, 2005, Liverpool, UK.
35. István Fábián, Gábor Lente (lecture)
Activation parameters in solution kinetics: use, misuse, and abuse
34th Inorganic Reaction Mechanisms Group Annual Meeting, January 5-7, 2005, Liverpool, UK.
34. Gábor Lente (lecture in Hungarian)
Királis autokatalízis: egy példa a sztochasztikus kinetika alkalmazására (Chiral autocatalysis - an example of using stochastic kinetics)
Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, October 28-29, 2004, Gyöngyöstarján, Hungary.
33. Ildikó Kerecsi, Gábor Lente, István Fábián (lecture in Hungarian)
Szulfition fotoiniciált és jodidion-katalizált autooxidációja (Photoinitiated and iodide ion catalyzed autoxidation of sulfite ion)
Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, October 28-29, 2004, Gyöngyöstarján, Hungary.
32. Katalin Ósz, Gábor Lente, Csilla Kállay (poster)
New protonation microequilibrium treatment in the case of some amino acid and peptide derivatives containing bis(imidazolyl)methyl group
7th European Biological Inorganic Chemistry Conference, August 29 - September 2, 2004, Garmisch-Partenkirchen, Germany.
31. István Fábián, Viktor Csordás, Gábor Lente (lecture in Hungarian)
Összetett reakcióelegyek kinetikai diszkrimináción alapuló analízise (Analysis of Complicated Reaction Mixtures Based on Kinetic Discrimination)
Chemistry Conference 2004, June 30 - July 2, 2004, Balatonföldvár, Hungary.
30. Katalin Ósz, Gábor Lente, Csilla Kállay (lecture in Hungarian)
Új számolási módszer kis molekulák protonálódási mikroállandóinak a

meghatározására (Novel Method for the Determination of Protonation Microequilibrium Constants of Small Molecules)
39th Colloquium on Coordination Chemistry, May 26-28, 2004, Gárdony, Hungary.

29. Gábor Lente, James H. Espenson (lecture in Hungarian)
Vastartalmú komplexek katalitikus hatásának vizsgálata 2,4,6-triklórfenol teljes kémiai lebontásában (A Study of the Catalytic Effect of Iron Complexes on the Complete Chemical Degradation of 2,4,6-Trichlorophenol)
39th Colloquium on Coordination Chemistry, May 26-28, 2004, Gárdony, Hungary.

28. Gábor Lente (lecture in Hungarian)
Klórfenolok katalitikus oxidációja hidrogén-peroxiddal - kezdeti lépések (Catalytic oxidation of chlorophenols by hydrogen peroxide - initial steps)
Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, April 29-30, 2004, Balatonalmádi, Hungary.

27. Ildikó Kerezsi, Gábor Lente, István Fábián (lecture in Hungarian)
Szulfition fotoiniciált és cérium(III)-katalizált autooxidációja (Photoinitiated and cerium(III)-catalyzed autoxidation of sulfite ion)
Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, April 29-30, 2004, Balatonalmádi, Hungary.

26. Gábor Lente, Ildikó Kerezsi, István Fábián (poster)
Reaction of the iron(III) hydroxo dimer with periodate ion
Inorganic Reaction Mechanisms Meeting, January 8-10, 2004, Athens, Greece.

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A 2,6-diklóorkinon fotoredukciója vizes oldatban - diódasoros spektrofotométer használata fotokémiai reakciók tanulmányozására (Photoreduction of 2,6-dichloroquinone in aqueous solution - use of a diode array spectrophotometer to study photochemical reactions)
Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, October 30-31, 2003, Gyöngyöstarján, Hungary.

24. Gábor Lente, James H. Espenson (lecture)
Photooxidation of water by 2,6-dichloro-1,4-benzoquinone
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23. Gábor Lente, James H. Espenson (poster)
Kinetics and Mechanism of the Oxidation of 2,4,6-Trichlorophenol by Hydrogen Peroxide Catalyzed by a Water-Soluble Iron(III) Porphyrin
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22. Gábor Lente, István Fábián (lecture)
Reactions of the Dithionate Ion: Disproportionation and Oxidation
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21. Ildikó Kerecsi, Gábor Lente, István Fábián (lecture in Hungarian)
A vas(III) hidroxodimer reakciója perjudátiókkal (Reaction of the iron(III) hydroxo dimer with periodate ion)
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19. Gábor Lente, István Fábián (lecture in Hungarian)
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18. Gábor Lente, István Fábián (invited presentation)
Kinetic modelling of the iron(III) – sulfite ion reaction at iron(III) excess
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17. Gábor Lente, István Fábián (lecture in Hungarian)
A vas(III) hidroxodimer reakciói egyszerű szerves anionokkal (Reactions of the iron(III) hydroxo dimer with simple inorganic anions)
36th Colloquium on Coordination Chemistry, May 23-25, 2001, Pécs, Hungary.
16. Gábor Lente, István Fábián (lecture)
Reactions of the hydrolytic iron(III) dimer $\text{Fe}_2(\mu\text{-OH})_2(\text{H}_2\text{O})_8^{4+}$ with simple inorganic oxoanions
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15. Gábor Lente, István Fábián (lecture in Hungarian)
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Highly labile sulphito complexes of chromium(III)
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13. Zsuzsa Hadady, Gábor Lente, István Fábián (lecture in Hungarian)
Vas(II)ion gyors képződésének követése szelektív kinetikai detektálással (Monitoring of fast formation of iron(II) with selective kinetic detection)
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12. Gábor Lente, James H. Espenson (lecture in Hungarian)
A [(o-SC₆H₄CH₂S)(CH₃)Re^VO]₂ dimer monomerizációjának mechanizmusa

(Mechanism of monomerization of the dimer $[(o\text{-SC}_6\text{H}_4\text{CH}_2\text{S})(\text{CH}_3\text{Re}^{\text{V}}\text{O})_2]$)
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11. Gábor Lente (lecture in Hungarian)

Új metil(oxo)rénium(V) komplexek reakciói (Reactions of novel methyl(oxo)rhenium(V) complexes)

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10. Gábor Lente, James H. Espenson (poster)

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9. István Fábián, Gábor Lente, Attila Nemes, Zsuzsanna Tóth (lecture in Hungarian)

Reaktív köztitermékek egyszerű szervesetlen vegyületek redoxireakcióiban

(Reactive intermediates in the redox reactions of simple inorganic compounds)

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8. Gábor Lente, István Fábián (poster)

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Középiskolákban tartott kémianépszerűsítő előadások

A 2000. évi tisztai ciánszennyezés kémiai háttere

2006. március 23., Hőgyes Endre Gimnázium, Hajdúszoboszló

Nemesfémek és drágakövek

2006. május 2., Hőgyes Endre Gimnázium, Hajdúszoboszló

A periódusos rendszer története és jövője

2006. szeptember 26., Hőgyes Endre Gimnázium, Hajdúszoboszló

Nukleáris balesetek

2007. március 1., Hőgyes Endre Gimnázium, Hajdúszoboszló

Nemesfémek és drágakövek

2007. október 24., Erdey-Grúz Tibor Vegyipari és Környezetvédelmi Szakközépiskola,
Debrecen

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Don't Be Tricked by Your Integrated Rate Plot: Pitfalls of Using Integrated Rate Plots

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amplification of ee cannot occur. This result is noteworthy, because it was recently shown by Lente (33) in a discrete modeling approach that a final ee $\neq 0$ can be obtained with the same autocatalytic model but omitting the mutual inhibition step. However, there is no contradiction between this result and ours because this discrepancy is only apparent. In the discrete approach, there is no amplification of ee at all because the reproduction of a *unique* molecule is considered and, obviously, a single chiral molecule always is enantiopure. Our deterministic simulations of model 1 can also generate this effect by taking appropriate parameter values in accordance with the simulations of Lente.^{||}

^{||} $k_2 = 0$, $[R]_0 = 1.66 \times 10^{-24}$ M, i.e., $1/N_A$ (Avogadro's number) for a unique molecule, and $k_0/k_1[A]_0 < 10^{-23}$. Remarkably, such a value fits well the Lente parameter $\alpha_L = k_1/k_0N_A V$ (V , sample volume) in which mirror-symmetry breaking occurs at $\alpha_L > 0.5$. Using the relationship $k_0/k_1[A]_0 = 1/(\alpha_L N_A V[A]_0)$, one arrives at $k_0/k_1[A]_0 < 10^{-23}$.

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In the absence of recycling ($\lambda = 0$), there is no reason that the final probability distribution takes the form given by the detailed balance condition, because there is no back reaction to balance with the production, but it is interesting to examine P_f in the limit $\lambda \rightarrow 0$. Since all the substrate molecules turn into chiral products, N_A should be zero so that $P_f(N_A > 0, N_R, N_S) = 0$. Thus, the final state lies on a fixed line $r + s = c$ or $N_R + N_S = N$. The probability (27) in this limit takes a binomial distribution along the fixed line as

$$P_f(0, N_R, N - N_R) = \frac{N!}{N_R!(N - N_R)!} \left(\frac{1}{2}\right)^N. \quad (30)$$

This result is identical with the solution obtained by Lent, who analyzed the same system with no recycling assuming a complete achiral state $(N, 0, 0)$ as the initial condition.^{29,30}

In fact, for $\lambda \rightarrow 0$, eq. (17) tells us that the final probability is nonzero only along the fixed line $N_A = 0$, or $N_R + N_S = N$, in the N_R - N_S phase space, and the normalized probability is calculated explicitly as

$$\begin{aligned} & P_f(0, N_R, N - N_R) \\ &= \frac{N!}{N_R!(N - N_R)!} \frac{f(k_0, \kappa_1, 0; N_R) f(k_0, \kappa_1, 0; N - N_R)}{f(2k_0, \kappa_1, 0; N)}. \end{aligned} \quad (32)$$

This result is again identical with the solution obtained by Lent, starting from the complete achiral state $(N, 0, 0)$.^{29,30}

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Activation Parameters. Standard enthalpies and entropies of activation were computed for all of the 25 chlorination reactions from the individual temperature dependence of their rate constants in terms of the Eyring equation written in the form of eq 5. As Lente et al.⁴² commented recently, $\Delta^\ddagger S^\circ$ values calculated from the best fitting parameters in eq 5 are as reliable as the corresponding $\Delta^\ddagger H^\circ$ values. These activation parameters

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J|A|C|S
ADDITIONS AND
CORRECTIONS

The Chlorate–Iodine Clock Reaction [*J. Am. Chem. Soc.* **2005**, *127*, 18022–18023]. André P. Oliveira and Roberto B. Faria*

Recent results on the chlorate–iodine clock reaction (Galadja, M.; Lent, G.; Fábian, I. *J. Am. Chem. Soc.* **2007**, *129*, 7738–7739) demonstrate that the reaction is initiated by UV light from the deuterium lamp employed in the diode-array spectrophotometer. These authors have shown that the UV light dissociates I₂, forming I* radicals that start the autocatalytic clock behavior. We did not consider the effect of light in our original mechanistic interpretation. Based on these new results, the chlorate–iodine reaction is the first example of a clock reaction induced by light, and the mechanism proposed by Galadja, Lent, and Fábian must be used to explain this clock reaction.

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other aromatics (21, 22). Lente and Espenson summarized different iron-based catalysts using H_2O_2 as a sole oxidant, which have 4 N donor atoms in a planar arrangement surrounding the metal center (23). It should be emphasized

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Stochastic Fluctuations and Chiral Symmetry Breaking: Exact Solution of Lente Model†

Jiushu Shao*‡§ and Lan Liu§

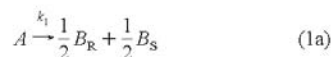
College of Chemistry, Beijing Normal University, Beijing 100875, China, and Institute of Chemistry, Chinese Academy of Sciences, Beijing 100080, China

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The stochastic description for the autocatalytic process has been proposed by Lente (*J. Phys. Chem. A* **2004**, *108*, 9475) to demonstrate chiral symmetry breaking. He assumed that the number of reacting molecules is macroscopic and that no products are present initially. The Lente model consisting of a finite number of molecules that may include the product molecules as chiral seeds is explored and the characteristics of stochastic distributions of the product are examined. It is shown that the presence of racemic product in the substrate reduces the possibility of chiral symmetry breaking while a few more molecules of a specific enantiomer added can yield chiral dominance for strong autocatalysis. Besides, small reactive volumes or dense reactant concentrations have a preference for chiral symmetric breaking.

Several kinetic models were suggested for chiral symmetry breaking in crystallization and Soai reaction,^{6,9} but the proposed mechanisms are far from conclusive. Recognizing the particulate feature of molecules, Lente put forward a stochastic model to explain the chiral symmetry breaking in autocatalytic reactions.¹⁰ He considered the case where no chiral product exists at the beginning of the reaction and used the cumulative distribution function as the quantity for experimental verification. In fact, when the number of molecules becomes small, the deterministic theory of chemical kinetics is no longer valid, and the stochastic theory characterizing the indeterministic behavior for the individual molecules should be used to describe the dynamical processes. An extreme example is a prochiral reaction with one reactant molecule in the container. Without any chiral influences, the very one molecule produced must randomly choose a specific configuration between its two enantiomers. One may think that as the number of molecules becomes macroscopic, the racemic product is most dominant. This, as shown in ref 10 is only true when the autocatalysis is very weak and asymmetric outcomes are the most probable for sufficiently strong autocatalysis.

The stochastic model needs to be further explored. In particular, because it is the particulate feature of molecules that makes the chemical reactions intrinsically stochastic, to reveal the interplay between the number of molecules the presence of chiral product and the symmetry breaking, which has not been examined in ref 10, is desired. To this end, we define direct statistical measures for experiments and analyze how the initial product molecules control the chiral yields. We start with the prochiral reaction with autocatalysis, which is well described by the following steps¹⁰



To summarize, we have studied the Lente model in a general case and have derived the exact expression for the mean and standard deviation of the ee value for the chiral product. It is observed that racemic product added in the reaction is detrimental to chiral symmetry breaking while the presence of chiral seeds helps enantioselectivity. The relationship between the

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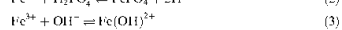
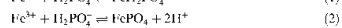
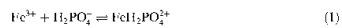
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carbon) removal rate was constant over 5.5 mM Oxone [29,30]. These trends are similar to the pattern observed in our study. The reason could be the radical scavenging effect which competes with PCP and reduce the reaction rates. In a previous study on the degradation of 2,4,6-trichlorophenol by H₂O₂ and Oxone using complex iron activators based on ligands of nitrogen. Lente et al. [33] reported the formation of Cl⁻ in the primary reaction and Oxone oxidizing it to chlorine gas under catalytic conditions. This reaction is not desirable as it consumes oxidizing agent and generates a toxic gas. The consumption of oxidant could be the possible reason for the reduced rates with Oxone and UV in our study.

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The UV/Vis measurements carried out on the flutriafol working solution showed change in the absorbance spectra of flutriafol during contact with ZVI. However, this observation is perceptible just at the beginning of the experiment ($t < 15$ min) before the formation of a high concentration of iron phosphate complex ($t > 15$ min) masking the absorbance of all by-products. This complex presents two broad absorption bands extending from 280 to 240 nm and from 240 to 194 nm, respectively with a maximum at 275 nm. The iron phosphate complex is attributed to the formation of $\text{FeH}_2\text{PO}_4^{2+}$ and FePO_4 summarized as follows (Lente et al., 2000):



All the above-mentioned equations most probably occur in our experimental conditions but at different rates. For example, the metal cations (Fe^{3+}) hydrolysis reactions (Eqs. (3) (5)) should take place at a very high rate if the solution was free of phosphate; however, in the presence of phosphate anions, the hydrolysis reaction decreases while iron phosphate complex formation increases (Eqs. (1) and (2)). As the reaction progresses, ferric cations are produced at the same time as their complexation with phosphate anions to form $\text{Fe}_4\text{P}^{\text{V}}$, a tetranuclear iron phosphate complex (Lente et al., 2000).

Lente, G., Magalhães, M.E.A., Fábian, J., 2000. Kinetics and mechanism of complex formation reactions in the iron(III) phosphate ion system at large iron(III) excess. Formation of a tetranuclear complex. *Inorg. Chem.* **39**, 1950-1954.

EXAMPLE OF A DETERMINISTIC MECHANISM:
PARITY VIOLATION

It has been argued that a parity-violating force such as interaction of the valence and core electrons with the atomic nuclei by the weak force can cause a small energy difference ΔE_{pv} between two enantiomers. This energy difference has been calculated for amino acids and sugars (see e.g. the discussion in¹²). Values range around $\Delta E_{pv} = 10^{-13} \text{ J mol}^{-1}$,^{13,14,24-26} which is $4 \times 10^{-17} k_B T$ for T near room temperature. In equilibrium, the relative concentrations (probabilities p and q) of the two isomers will then deviate from 0.5 by $\pm \varepsilon$, with

$$\varepsilon = \Delta E_{pv}/4k_B T = 10^{-17} \quad (3)$$

as derived by Lente,²⁷ for example. To judge whether ε is statistically significant, Lente²⁷ derives and calculates a function $R(N)$, the excess probability for formation of the more stable enantiomer; it is illustrated in Figure 1. He finds that R reaches a sufficiently high level (0.2–0.5) only, if the total ensemble comprises $N = 10^{32}$ – 10^{33} molecules. This seems an unreasonably large number of initial molecules (amino acids are assumed in²⁷; see, however, Section Homochirality probably originates from RNA-like oligomers, not from small molecules), from which life would have emerged. Lente concludes that even if ΔE_{pv}

were 3–4 orders of magnitude larger, parity violation could not have caused homochirality.²⁷

I would like to use a more direct argument, which leads to the same conclusion without much calculation: An enantiomer excess ee predicted by parity violation as small as $ee = 2\varepsilon = 2 \times 10^{-17}$ is *smaller than the standard deviation* expected due to the statistics of an ensemble of up to $N \leq 0.25 \times 10^{34}$ molecules (eq. 2), *the discrepancy becoming larger for smaller N* . Generally, one deduces from eq. 2 the minimum number of molecules N_{\min} , which is required for any deterministic mechanism to be competitive with the chance mechanism in producing a relative enantiomeric excess ee

$$N_{\min} = (ee)^{-2} \quad \text{or} \quad N_{\min} = 0.25\varepsilon^{-2} \quad (4)$$

If $N < N_{\min}$, the ee expected from the chance mechanism ($ee = 2\sigma/N$) will be larger than the deterministic ee ($ee = 2\varepsilon$), and *any detected ee must in this case be considered accidental*. In this case, the envisaged deterministic effect is not statistically significant. The cases $N < N_{\min}$ and $N \approx N_{\min}$ are shown in Figs. 1a and 1b.

It may be helpful to illustrate these statements further. The number $N_{\min} = 2.5 \times 10^{33}$ given above for the parity-violation mechanism would correspond to about $(2.5\text{--}6) \times 10^{10}$ kg of a self-replicating molecule, if this is assumed to be a short-chain RNA with about 20–50 bases. This can be compared with the contents of a pore, which is discussed as the probable location of the emergence of self-replicating systems.^{1,2,8,28,29} So, even if the magnitude of ΔE is as large as calculated (for doubts, in particular also caused by the conformer dependence, see^{9,14,25,26,30} and also the discussion in¹²) or several orders of magnitude larger, *one should not consider the parity-violating force a cause of biological homochirality*. Fluctuations of a different kind (in subsequent chirality-amplification reactions) have already in 1975 been invoked against an importance of parity violation.³¹ Very recently, Lente extended his statistical treatment, considering now also such subsequent autocatalytic reactions.³² He finds that then N_{\min} becomes even much more unrealistic.

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Lente proposed a discrete-state stochastic modeling approach in which chiral amplification could be described by a quadratic autocatalytic model without considering cross-inhibition [67, 68]. However, the discrepancy between the usually employed deterministic kinetic approach, which reinforces the need for cross-inhibition, and the discrete-state stochastic approach is only apparent. The discrete approach considers the repetitive reproduction of single molecules which, in the case of a chiral system, obviously are individually all enantiomerically pure. Hence, basically no amplification of the *ee* occurs at all during the discrete scenario. It has been indicated that deter-

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