UNIVERSITY OF PÉCS

Doctoral School of Chemistry

Interaction between aniline derivatives and single-walled carbon nanotubes investigated by fluorescence and quantum-chemical methods

PhD Thesis

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1. Introduction

The Carbon Nanotubes (CNTs) have been found attractive material in materials science due to its applicability in wide scale of industrial usages. At the same time their widespread application in chemistry, biochemistry, biology and medicine is hindered by their low solubility in aqueous or most organic and inorganic media. The carbon nanotubes are soluble only in a few low permittivity solvents, which property makes impossible the study of several important phenomena, *e.g.* investigation of the tubular ion-transport by electrochemical methods. Accordingly, the CNTs solubilised in aqueous or organic media have attracted increased attention. Two approaches are known to solubilize or disperse the CNTs: one is the chemical modification of CNTs by covalent bonding and the other one is the physical modification by noncovalent functionalization.

American researchers have shown that it is possible to dissolve single-walled carbon nanotubes (SWCNTs) in aniline solvent. In spite of the increased attention, the detailed solvation mechanism was not clarified yet. According to the theory described by Sun *et al.*, the aniline itself can solve the nanotubes by forming a soluble charge-transfer complex. However, due to the high concentration of aniline and considering its low permittivity, it is obvious to assume the presence of π-π interaction between the aromatic rings of the aniline and the nanotube. The interactions between molecules containing π-electron-systems was described in detailed earlier since this interaction play important role in several biological and chemical processes. The effects of the solvent permittivity on the stability of the π-π interaction between aromatic molecules were clearly determined before.

2. Objectives

The main aim of this work was to understand the solvation mechanism of carbon nanotubes in aniline solvent. To clarify the solvation mechanism the part of the experimental analysis was extended for investigation of the dissolution of carbon nanotubes in some aniline derivatives too. The effect of the permittivity of the molecular environment on the weak interactions between carbon nanoubes and aniline derivatives was also studied, furthermore the adsorption properties of aniline on the surface of SWCNTs and the thermodynamics of solubilization of SWCNTs were investigated. Quantum chemical calculations were performed to describe the solvation process at molecular level. During this analysis the solvent effect on the aniline – SWCNT interaction and the relationship between the optical and structural properties of the complex were studied.

3. Methods

The experimental work was done using the Fluorolog τ3 spectrofluorimeter (Jobin-Yvon/Spex) and the Nicolet NXR 5700 FT–IR–Raman (UNICAM) photometer. During the theoretical investigation the quantum chemical analysis were done by GAUSSIAN 03 Rev.B.05. and by TURBOMOLE 5.7.1. program packages, the molecular dynamics simulations were carried out by HyperChem Professional 7 software package.

4. Results

In this work the solubilization of single-walled carbon nanotubes has been investigated by fluorescence and quantum-chemical methods. In this frame the permittivity dependence of the interaction between the nanotube and aniline were examined in detail. The following statements were established by these investigations:

1. The solubility of carbon nanotubes in aniline solutions has been determined. Results show much lower dissolution of SWCNTs in aniline compared to it published earlier. Accordingly, only 0.001 mg SWCNTs can be dissolved in 1 ml aniline.
2. The earlier published solubilization process is based on the formation of charge – transfer complex between the aniline molecules and the nanotube. Applying aniline derivatives which possess $-CH_3$ groups at appropriate sites, the formation of charge transfer complexes was inhibited, therefore we were able to study the role of π-π interaction in the solubilization separately. The results highlighted the complex behavior of the aniline – nanotube interaction and enhanced role of the π-π interaction between the aromatic rings of aniline and that of the nanotubes has been determined.
3. The fluorescence spectra observed after alcoholic dilution of solutions of aniline – SWCNT, 2,6-dimethyl-aniline – SWCNT and *N,N*-dimethyl-aniline – SWCNT reflect significant changes in the molecular environment around the nanotube. The spectral changes suggest that the co-solvent alcoholic molecules also participate in the solubilization processes.
4. The free-enthalpy change associated to the aniline – nanotube interaction was found lower than it was observed earlier according to the π-π interaction of other aromatic molecules. However, same trend was observed in the permittivity dependence of the interaction: stronger aniline – nanotube interaction was detected in low-permittivity solvents.

5. We have shown that the BP86-D and in some cases the MPWB1K sets are appropriate functionals to describe the aniline – nanotube interactions. Aniline – $C_{42}H_{16}$ (n,0) SWCNT fragment, or aniline – $C_{64}H_{20}$ (n,0) SWCNT fragment + 2 MeOH (n=8, 10 or 30) systems were applied to represent the interacted species. Unfortunately, the theoretical results cannot be directly comparable with the experiments due to the limited size of the fragments.

6. The calculated adsorption energies validate that the stacked π-π structures are more stable than the T-shaped structures. The results of the DFT calculations show that the top orientation of the aniline to the nanotube surface is responsible for the energetically most favorable conformation.

7. Our results suggest that under the change of the molecular environment both the conformation of the aniline – nanotube complex and the molecular skeleton of the aniline are changed significantly.

8. The results of the TDDFT calculations were compared with the experimental spectra. Although the experimental spectra don't show considerable changes in their shape, nor in their site during alcoholic dilution of the samples, the theoretical analysis validates appearance of weak new electronic transitions. However, these transitions don't result considerable change in the calculated spectra since their weakness.

9. A time-dependent deformation of the cross section of nanotube has been obtained by molecular dynamics simulations. This result prefers adsorption of such molecules on the surface of nanotube which have flexible molecular skeleton and/or possess flexible moieties.

We hope that our findings can contribute in the development of methods towards improving the solubility of nanotubes and can improve efficiently the applications of aromatic molecules in molecular packing.

5. List of publications

I. Publications in refereed journals related to these thesis

1. **B. Peles-Lemli**, L. Kollár, S. Kunsági-Máté:
   Thermodynamics of the solvation of carbon nanotubes: exchange of aniline to primary alcohols on the surface of carbon nanotubes
   Fullerenes, Nanotubes and Carbon Nanostructures (2010) in press IF= 0.680

2. **B. Peles-Lemli**, G. Matisz, A.-M. Kelterer, W.M.F. Fabian, S. Kunsági-Máté:
   Non-covalent Interaction Between Aniline and Carbon Nanotubes: Effect of Nanotube Diameter and the Hydrogen-bonded Solvent Molecules on the Adsorption Energy and the Photophysics.
   Journal of Physical Chemistry C 114 (2010) 5898-5905. IF=3.396

3. **B. Peles-Lemli**, P. Ács, L. Kollár, S. Kunsági-Máté:
   Permittivity-dependent carrier behavior of aniline derivatives towards common low-permittivity solvents in the solubilization of carbon nanotubes
   Fullerenes, Nanotubes and Carbon Nanostructures 16 (2008) 247-257. IF= 0.680

4. **B. Peles-Lemli**, J. Peles-Lemli, L. Kollár, G. Nagy, S. Kunsági-Máté:
   Temperature-independent longitudinal waves obtained on carbon nanotubes with special emphasis on the tubular ion-transport
   Studia Universitatis Babes-Bolyai, Seria Chemia 2 (2008) 37-41. IF=0.000

II. Publications in non-refereed journals, conference abstarcts, lectures and posters related to these thesis

II.a Non-refereed publications and conference abstracts in full

1. **B. Peles-Lemli**, S. Kunsági-Máté:
   Szén nanocsövek rezgéseinek tanulmányozása elméleti kémiai módszerekkel - NIIF szuperszámítógép a nanotechnológiában
   NIIF Hírlevél (Publisher: Miklós Nagy, director of the Hungarian National Infrastructure Development Program Office, Editor: Tamás Máray, ISSN 1588–7316) 4(2) 2007 pp. 9

2. **B. Peles-Lemli**, P. Ács, L. Kollár, G. Nagy, S. Kunsági-Máté:
   A molekulakörnyezet permittivitásának hatása szén nanocsövek és aromás molekulák gyenge kölcsönhatására
   Műszaki Kémiai Napok ’07, (Pannon University, Veszprém (Hungary), Editor: Endre Nagy, ISBN 978 963 9696 15 0), 2007 pp. 253-257.

3. **B. Peles-Lemli**, J. Peles-Lemli, L. Kollár, G. Nagy, S. Kunsági-Máté:
   Szén nanocsövekben megvalósuló, iontranszportot meghatározó karakterisztikus rezgések és ezek meglepő hőmérsékletfüggése
   Műszaki Kémiai Napok ’07, (Pannon University, Veszprém (Hungary), Editor: Endre Nagy, ISBN 978 963 9696 15 0), 2007 pp. 262-265.

II.b International conference abstracts, lectures and posters

1. **B. Peles-Lemli**, W.M.F. Fabian, A.-M. Kelterer, L. Kollár, S. Kunsági-Máté:
   Weak Interactions of Aromatic Compounds Regarding the Solvation Mechanisms of Aniline-Carbon Nanotube Aggregates in Alcoholic Solutions
   10th International Conference on Calixarenes, Korea University, Seoul, South Korea, 13-16 July, 2009., P129

2. **B. Peles-Lemli**, W.M.F. Fabian, A.-M. Kelterer, S. Kunsági-Máté:
   Adsorption of aniline derivatives on carbon nanotube as key step towards permittivity-dependent solubilisation
   Molecular Modelling in Chemistry and Biochemistry (MOLMOD 2009), Cluj-Napoca (Romania) 2-4 April 2009

3. **B. Peles-Lemli**
   The role of the solution permittivity in the solubilization of anilin – carbon nanotubes in common solvents
   DissertantInnenseminar in Chemie III (LV 646.516) at Institute of Chemistry (IfC) of the Karl-Franzens University, Graz (Austria), 23 January 2009.

4. **B. Peles-Lemli**, P. Ács, L. Kollár, S. Kunsági-Máté:
   The role of the solution permittivity in the stability of aniline – SWCNT interaction in alcoholic solvents
   Nanotechnology Materials and Devices Conference 2008, Kyoto (Japan), 20-22 October 2008.

5. **B. Peles-Lemli**, W.M.F. Fabian, S. Kunsági-Máté:
   Adsorption of aniline molecule on the planar and rolled graphene surfaces due to its role in the solubilization of carbon nanotubes
   44th Symposium on Theoretical Chemistry, From Basic Principles to Applications, Ramsau am Dachstein (Austria), 23-27 September 2008.

6. **B. Peles-Lemli**, L. Kollár, G. Nagy, S. Kunsági-Máté:
   The effect of vibration dynamics of SWCNTs on their ion and molecule transport
   9th Symposium on Instrumental Analysis, Pécs (Hungary), 29 June - 2 July 2008.

7. **B. Peles-Lemli**, P. Ács, L. Kollár, S. Kunsági-Máté:
   Solubilization of SWCNTs: Permittivity-dependent carrier property of aniline derivatives
   9th Symposium on Instrumental Analysis, Pécs (Hungary), 29 June - 2 July 2008.

8. **B. Peles-Lemli**, P. Ács, L. Kollár, G. Nagy and S. Kunsági-Máté:
   The effect of solvent permittivity on the weak interaction between carbon nanotubes and aromatic molecules
   3rd International Conference on Optoelectronics and Spectroscopy of Nano-structured Thin Films and Materials, Beijing (China), Capital Normal University, 15-19 October 2007.

9. **B. Peles-Lemli**, J. Peles-Lemli, L. Kollár, G. Nagy and S. Kunsági-Máté:
Effect of dynamical motions of carbon nanotubes on the ion-transport behavior and their solubilization processes
3rd International Conference on Optoelectronics and Spectroscopy of Nano-structured Thin Films and Materials, Beijing (China), Capital Normal University, 15-19 October 2007.

10. **B. Peles-Lemli**, J. Peles-Lemli, L. Kollár, G. Nagy, S. Kunsági-Máté:
Temperature-independent longitudinal waves obtained on carbon nanotubes with special emphasis on the tubular ion-transport
Molecular Modelling in Chemistry and Biochemistry (MOLMOD 2007), Arcalia (Romania) 5-8 July 2007

11. **B. Lemli**, J. Peles, L. Kollár, G. Nagy, S. Kunsági-Máté
Molecular dynamics study of single-walled carbon nanotubes in accordance to their solubilization
1st European Chemistry Congress, Budapest (Hungary), 27-31 August 2006.

II.c National conference abstracts, lectures and posters

1. **B. Peles-Lemli**, P. Ács, L. Kollár, G. Nagy, S. Kunsági-Máté
Az oldószer permittivitásának hatása szén nanocsövek oldhatóságára
Centenáriumi Vegyészkonferencia (Centenary Chemist Conference), Sopron, (Hungary), 29 May – 1 June 2007

2. **B. Peles-Lemli**, J. Peles-Lemli, L. Kollár, G. Nagy, S. Kunsági-Máté
Szén nanocsövek karakterisztikus rezgései és a dinamikai tulajdonságok hőmérsékletfüggése
Centenáriumi Vegyészkonferencia (Centenary Chemist Conference), Sopron, (Hungary), 29 May – 1 June 2007

3. **B. Peles-Lemli**, P. Ács, L. Kollár, G. Nagy, S. Kunsági-Máté
Szén nanocsövek és anilin származékok molekuláris rezgéseinek szerepe a szolvatáció folyamatában
Centenáriumi Vegyészkonferencia (Centenary Chemist Conference), Sopron, (Hungary), 29 May – 1 June 2007

4. **B. Peles-Lemli**, P. Ács, L. Kollár, G. Nagy, S. Kunsági-Máté:
A molekulakörnyezet permittivitásának hatása szén nanocsövek és aromás molekulák gyenge kölcsönhatására
Műszaki Kémiai Napok ’07 (Conference of Chemical Engineering ’07) Veszprém , (Hungary), 25-27 April 2007

5. **B. Peles-Lemli**, J. Peles-Lemli, L. Kollár, G. Nagy, S. Kunsági-Máté:
Szén nanocsövekben megvalósuló, iontranszportot meghatározó karakterisztikus rezgések és ezek meglepő hőmérsékletfüggése
Műszaki Kémiai Napok ’07 (Conference of Chemical Engineering ’07), Veszprém , (Hungary), 25-27 April 2007

6. **B. Lemli**, J. Peles, L. Kollár, G. Nagy, S. Kunsági-Máté
Szén nanocsövek adszorpcióképességének vizsgálata
II. Kárpát-medencei Környezettudományi Konferencia (II. Conference on Environmental Sciences of the Carpathian Basin), Pécs, (Hungary), 1-3 June 2006

7. **B. Lemli**, J. Peles, L. Kollár, G. Nagy, S. Kunsági-Máté
Szén nanocsövek rezgési tulajdonságai
Műszaki Kémiai Napok '06 (Conference of Chemical Engineering '06), Veszprém (Hungary), 25-27 April 2006

III. Other publications in refereed journals

1. **B. Peles-Lemli**, J. Peles-Lemli, I. Bitter, L. Kollár, G. Nagy, S. Kunsági-Máté:
Competitive Thermodynamic and Kinetic Processes During Dissociation of Some Host-Guest Complexes of Calix[4]arene Derivatives
Journal of Inclusion Phenomena and Macrocyclic Chemistry 59(3-4) (2007) 251-256. IF=1.153

2. **B. Lemli**, J. Peles, L. Kollár, G. Nagy, S. Kunsági-Máté:
The rate of host-guest complex formation of some calixarene derivatives towards neutral aromatic guests
Supramolecular Chemistry 18(03) (2006) 251-256. IF=1.861

3. S. Kunsági-Máté, K. Szabó, **B. Lemli**, I. Bitter, G. Nagy, L. Kollár:
Host-guest interaction between water-soluble calix(6)arene hexasulfonate and p-nitrophenol
Thermochimica Acta 425(1-2) (2005) 121-126. IF=1.230

4. **B. Lemli**, L. Kollár, G. Nagy, G. Molnár, S. Kunsági-Máté:
The predective behavior of the phase transition temperatures of imidazolium based ionic liquids
Lecture Series on Computer and Computational Sciences 4A (2005) 315-318. IF=0.000

5. S. Kunsági-Máté, K. Szabó, **B. Lemli**, I. Bitter, G. Nagy, L. Kollár:
Increased complexation ability of water-soluble calix(4)resorcinarene octacarboxylate towards phenol by the assistance of Fe(II) ions
Journal of Physical Chemistry B 108 (2004) 15519-15522. IF=3.834

6. S. Kunsági-Máté, **B. Lemli**, G. Nagy, L. Kollár:
Conformational change of the cation-anion pair of an ionic liquid related to its low-temperature solid state phase transitions
Journal of Physical Chemistry B 108 (2004) 9246-9250. IF=3.834

IV. Other publications in non-refereed journals, conference abstarcts, lectures and posters

IV.a Non-refereed publications and conference abstracts in full

1. S. Kunsági-Máté, K. Szabó, **B. Peles-Lemli**, J. Peles-Lemli, C. Schür, H.P. Strunk
   Fenolszármazékok adszorpciója GaAs(001) kristály felületén
   Műszaki Kémiai Napok '07, (Pannon University, Veszprém (Hungary), Editor: Endre Nagy, ISBN 978 963 9696 15 0), 2007 pp. 266-270.

2. J. Peles, **B. Lemli**, I. Bitter, L. Kollár, G. Nagy, S. Kunsági-Máté:
   Kalixarének aromás semleges molekulákkal alkotott komplexeinek meglepő disszociációs dinamikája
   Műszaki Kémiai Napok '06, (Pannon University, Veszprém (Hungary), Editor: Endre Nagy, ISBN 963 9495 86 7), 2006 pp. 173-176.

3. **B. Lemli**, L. Kollár, G. Nagy, S. Kunsági-Máté:
   Imidazólium kation alapú ionfolyadékok fázisátalakulásai
   XI. Nemzetközi Vegyészkonferencia, (Hungarian Technical Scientific Society of Transylvania, Editor: Kornélia Majdik, ISBN 973 7840 07 0), 2005 pp. 185-188.

4. J. Peles, **B. Lemli**, L. Kollár, G. Nagy, S. Kunsági-Máté:
   Kalixarének mint molekuláris kapszulák komplexeinek stabilitását meghatározó versengő termodinamikai és kinetikai folyamatok
   XI. Nemzetközi Vegyészkonferencia, (Hungarian Technical Scientific Society of Transylvania, Editor: Kornélia Majdik, ISBN 973 7840 07 0), 2005 pp. 198-201.

5. S. Kunsági-Máté, **B. Lemli**, G. Molnár, G. Nagy, L. Kollár:
   Imidazólium kation alapú ionfolyadékok fázisátmeneti hőmérsékleteinek tervezhetősége
   Műszaki Kémiai Napok '05, (Pannon University, Veszprém (Hungary), Editor: Endre Nagy, ISBN 963 9495 71 9), 2005 pp. 298-301.

IV.b International conference abstracts, lectures and posters

1. S. Kunsági-Máté, K. Szabó, B. Peles-Lemli, J. Peles-Lemli, C. Schür, H.P. Strunk
   Adsorption of phenol derivatives on GaAs(001) surfaces
   3rd International Conference on Optoelectronics and Spectroscopy of Nano-structured Thin Films and Materials, Beijing (China), Capital Normal University, 15-19 October 2007.

2. **B. Peles-Lemli**, J. Peles-Lemli, I. Bitter, L. Kollár, G. Nagy, S. Kunsági-Máté:
   The role of competitive thermodynamic and kinetic processes in the stabilization of host-guest complexes of calix[4]arene derivatives
   Molecular Modelling in Chemistry and Biochemistry (MOLMOD 2007), Arcalia (Romania) 5-8 July 2007

3. S. Kunsági-Máté, K. Szabó, **B. Peles-Lemli**, J. Peles-Lemli, C. Schür, H.P. Strunk:
   Molecular modelling of adsorption of phenols on GaAs(001) surface
   Molecular Modelling in Chemistry and Biochemistry (MOLMOD 2007), Arcalia (Romania) 5-8 July 2007

4. J. Peles, **B. Lemli**, I. Bitter, L. Kollár, G. Nagy, S. Kunsági-Máté
The stabilization of host-guest complexes of calixarene with neutral guests: competitive kinetic and thermodynamic processes
1st European Chemistry Congress, Budapest (Hungary), 27-31 August 2006.

5. **B. Lemli**, L. Kollár, G. Nagy, S. Kunsági-Máté
The phase transitions of imidazolium based ionic liquids
11th International Conference of Chemistry, Cluj (Romania), 11-13 November 2005.

6. J. Peles, **B. Lemli**, L. Kollár, G. Nagy, S. Kunsági-Máté
Competitive thermodynanic and kinetic processes determining the stability of complexes of calixarenes as molecular capsules
11th International Conference of Chemistry, Cluj (Romania), 11-13 November 2005.

7. **B. Lemli**, L. Kollár, G. Nagy, G. Molnár, S. Kunsági-Máté
The predective behavior of the phase transition temperatures of imidazolium based ionic liquids
International Conference of Computational Methods in Sciences and Engineering 2005 (ICCMSE 2005), Loutraki (Greece), 21-26 October 2005.

8. **B. Lemli**, S. Kunsági-Máté, G. Nagy, L. Kollár
Structural changes of cation-anion pair of the imidazolium-hexaflourophosphate ionic liquid with consequences on its solid-solid and solid-liquid phase transitions
8th Symposium on Instrumental Analysis, Graz (Austria), 25-28 September 2005.

9. **B. Lemli**, J. Peles, L. Kollár, G. Nagy, S. Kunsági-Máté
Effect of the tBu substituents of calixarene host molecules on the rate of host-guest formation with neutral aromatic guests
8th Symposium on Instrumental Analysis, Graz (Austria), 25-28 September 2005.

10. S. Kunsági-Máté, K. Szabó, **B. Lemli**, G. Nagy, L. Kollár
Guest – induced entropy compensation effect on the stability of the calix[6]arene – phenol host-guest complexes
8th Symposium on Instrumental Analysis, Graz (Austria), 25-28 September 2005.

11. **B. Lemli**, S. Kunsági-Máté, G. Nagy, L. Kollár
The rate of host-guest complex formation of some calixarene derivatives towards neural aromatic guests
8th International Conference on Calixarenes (CALIX2005), Prague (Czeh Republic), 25-29 July 2005.

12. S. Kunsági-Máté, **B. Lemli**, K. Szabó, G. Nagy, L. Kollár
Theoretical evaluation of the unusual entropy change during formation of calix[6]arene – phenol host-guest complexes
8th International Conference on Calixarenes (CALIX2005), Prague (Czeh Republic), 25-29 July 2005.

13. S. Kunsági-Máté, **B. Lemli**, G. Nagy, L. Kollár
Energetics of the proton tunneling channels related to the cyclic hydrogen bonds at lower rim of cone conformers of methyl-, thia- and oxa-calix[4]arenas
7th Symposium on Instrumental Analysis, Pécs (Hungary), 22-24 September 2003.

IV.c National conference abstracts, lectures and posters

1. S. Kunsági-Máté, K. Szabó, **B. Peles-Lemli**, J. Peles-Lemli, C. Schür, H.P. Strunk
Fenolszármazékok adszorpciója GaAs(001) kristály felületén
Műszaki Kémiai Napok '07 (Conference of Chemical Engineering '07), Veszprém , (Hungary), 25-27 April 2007

2. J. Peles, **B. Lemli**, I. Bitter, L. Kollár, G. Nagy, S. Kunsági-Máté
Szelektív kémiai érzékelésre alkalmas kalixarén származékok komplexképződési dinamikája
II. Kárpát-medencei Környezettudományi Konferencia (II. Conference on Environmental Sciences of the Carpathian Basin), Pécs (Hungary), 1-3 June 2006

3. J. Peles, **B. Lemli**, I. Bitter, L. Kollár, G. Nagy, S. Kunsági-Máté
Kalixarének aromás semleges molekulákkal alkotott komplexeinek meglepő disszociációs dinamikája
Műszaki Kémiai Napok '06 (Conference of Chemical Engineering '06), Veszprém (Hungary), 25-27 April 2006

4. **B. Lemli**
Környezeti szempontból kiemelkedő jelentőségű ionfolyadékok szerkezetváltozásainak vizsgálata
X. Országos Felsőoktatási Környezettudományi Diákkonferencia (X. National Higher Educational Environmental Science Student's Conference), Eger (Hungary), 10-12 April 2006.

5. S. Kunsági-Máté, **B. Lemli**, G. Molnár, G. Nagy, L. Kollár
Imidazólium kation alapú ionfolyadékok fázisátmeneti hőmérsékleteinek tervezhetősége
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6. **B. Lemli**
Ionfolyadékok szerkezetváltozásainak vizsgálata
XXVII. Országos Tudományos Diákköri Konferencia (XXVII. National Scientific Students' Associations Conference), Budapest (Hungary), 21-23 March 2005.

7. **B. Lemli**
Ionfolyadékok szerkezetváltozásainak vizsgálata
Tudományos Diákköri Konferencia, regionális forduló (Scientific Students' Associations Conference, regional round), Pécs (Hungary), 26 November 2004.

8. S. Kunsági-Máté, **B. Lemli**, G. Nagy, L. Kollár
Egy ionfolyadék meglepő szilárd-szilárd fázisátmenetének vizsgálata
Vegyészkonferencia 2004. (Chemist Conference 2004), Balatonföldvár (Hungary), 30 June – 2 July 2004.