Polskie Towarzystwo Chemiczne

Polish-Taiwanese Conference

From Molecular Modeling to Nano- and Biotechnology

MMNB 2014
4-6 Sept OPOLE

Organized by:

Department of Physical Chemistry and Molecular Modeling,

University of Opole, Opole, Poland

Tatung University, Taipei, Taiwan

Restauracja Hotel Villa Park, Opole

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conference logo: Dominik Tabisz
website: J.Hurek

INVITATION

Dear Colleagues,

on behalf of the organizing committee we have the pleasure to invite you to participate in

the Polish-Taiwanese Conference: "**From Molecular Modeling to Nano- and Biotechnology**".

The Conference will be held in Opole, Poland from September 4th to September 6th 2014 at ***the Villa-Park Opole-Groszowice and under the auspices of the Polish Chemical Society (PTChem), Taipei Economic and Cultural Office in Poland and the Self-Government of the Opole Voivodeship.***

The aim of our interdisciplinary meeting is to bring together specialists of molecular modeling and related fields of research working at the border of nanotechnology and biotechnology. Topics will cover all areas of basic and applied sciences.

The programme of the Conference will comprise full lectures (30 or 45 min.), oral communications (15 min.) and poster presentations. The official language of the Symposium is English.

We wish to encourage young scientists to attend the Conference and to present their own research on the special Young Scientists Session. The best contributions will be awarded. We consider active participation of young scientists to be the meeting's greatest asset.

WE ARE LOOKING FORWARD TO WELCOMING YOU IN OPOLE!

CONFERENCE COMMITTEES

Honorary Committee:

1. **Prof. dr hab. Stanisław S. Nicieja** *(Rektor, Opole University)*
2. **Prof. dr hab. inż. Piotr Wieczorek** *(Dean, Faculty of Chemistry, Opole University)*
3. **Prof. dr hab. inż. Krystyna Czaja** *(Head, Opole Section of Polish Chemical Society)*

Scientific Committee:

1. **Małgorzata Broda** *(University of Opole, Poland)*
2. **Gerd Buntkowsky** *(Technical University Darmstadt, Germany)*
3. **Frank Jensen** *(Aarhus University, Denmark)*
4. **Teobald Kupka** *(University of Opole, Poland)*
5. **Zdzisław Latajka** *(University of Wrocław, Poland)*
6. **Hong Ming Lin** *(Tatung Technical University, Taipei, Taiwan)*
7. **Volodymir Novikov** *(Lviv Polytechnic National University, Lvov, Ukraine)*
8. **Leszek Stobiński** *(Polish Academy of Sciences, Warsaw, Poland)*

Organizing Committee:

1. **Teobald Kupka** - chairman
2. **Hong-Ming Lin -** vice-chairman
3. **Marzena Jankowska (Nieradka) / Roksana Wałęsa / Aneta Buczek -** secretary
4. **Klaudia Radula-Janik** - member
5. **Michał Stachów** - member
6. **Monika Staś** - member

Invited speakers:

The following outstanding scientists have already accepted our invitation to deliver a lecture:

1. **Prof. Maria Barysz** *(Nicolaus Copernicus University, Toruń, Poland)*
2. **Prof. Gerd Buntkowsky** *(TU Darmstadt, Germany)*
3. **Prof. Yuh-Jing Chiou** *(Tatung University, Taipei, Taiwan)*
4. **Prof. Poul Erik Hansen** *(Roskilde University, Denmark)*
5. **Prof. Frank Jensen** *(Aarhus University, Denmark)*
6. **Dr. Jakub Kaminský** *(Czech Academy of Sciences, Prague, Czech Republic)*
7. **Dr. Tatiana Korona** *(Warsaw University, Poland)*
8. **Prof. Zdzisław Latajka** *(University of Wrocław, Poland)*
9. **Prof. Hong Ming Lin** *(Tatung University, Taipei, Taiwan)*
10. **Prof. Volodymir *Novikov*** *(Lviv Polytechnic National University, Lviv, Ukraine)*
11. **Prof. Riadh Sahnoun** *(Universiti Teknologi Malayisa, Skudai, Malaysia)*
12. **Prof. Szczepan Roszak** *(Wrocław Technical University, Poland)*
13. **Dr. Leszek Stobiński** *(Institute of Physical Chemistry, Warsaw, Poland)*
14. **Prof. Michal Straka** *(Czech Academy of Sciences, Prague, Czech Republic)*

Plenary lectures

1. **Frank Jensen**, “Recent trends in force field developments”.
2. **Gerd Buntkowsky**, "Applications of Solid State NMR on Nanocatalysts".
3. **Hong-Ming Lin**, “Magnetic Hyperthermia Effects of Functionalized Iron Nanowires”.
4. **Yuh-Jing Chiou**, “Synthesis and Characterization of Nano Hybrid MWCNTs Electrocatalysts”.
5. **Poul Erik Hansen**, “Hydrogen bonding - a key modeling parameter in nano and bio-systems”.
6. **Michal Straka**, "Endohedral Fullerenes with Actinide-Actinide Bonds: Unwilling Bonding in $U_2@C_{80}$".
7. **Tatiana Korona**, “Endohedral complexes of fullerenes and other large complexes - what can we get from contemporary ab initio methods?”.
8. **Jakub Kaminsky**, “Issues in modeling of Fullerenes”.
9. **Riadh Sahnoun**, "Encapsulation of hydrogen molecules inside selected fullerene cages: why the discrepancy between theoretical calculations and experimental results?" .
10. **Szczepan Roszak**, “Beryllium doping – the promising carbon modified materials”.
11. **Andrzej Bil**, “Modifying the Fullerene Surface Using Endohedral Light Guests. From Ab Initio Molecular Dynamics And Metadynamics To Quantum Chemical Topology”.

POSTERS AND LECTURES

Lectures

1. **Tadeusz Pluta, Miroslav Medved, Simon Budzak, Joanna Kauczor**, TDDFT determination of electric properties of excited states.
2. **Mariola Czuchry, Klemens Noga, Mariusz Sterzel**, Comprehensive support for chemistry in PL-Grid infrastructure.
3. **Wojciech Płonka**, "Quick and dirty modeling" – importance of simplifications in computational chemistry

Young scientists session:

1. **Monika Staś**, Conformational properties of non-standard amino acids with heterocyclic ring,
2. **Roksana Wałęsa,** Conformational properties of compounds with N-methylated peptide bond
3. **Marzena Jankowska (Nieradka),** Sensitivity of ^{21}Ne NMR parameters to nanoscopic systems
4. **Michał Stachów,** Teobald Kupka, and Farhod Nozirov, From Ethylene to plastic optical fiber

Posters

1. Grzegorz Bazgier and Jacek Lipok, Statistical computations enriching interpretation of FT-IR profiles of cyanobacteria - metabolomic approach **(P1)**

2. Artur Birczyński, Grzegorz Stoch, Zdzisław T. Lalowicz, Agnieszka Szymocha Kinga Góra-Marek, Jerzy Datka, Diverse dynamics of water molecules confined in cages of faujasites. Deuteron NMR investigation **(P2)**

3. D. Frączek, R. Wiśniowski, Applying of the lattice model to a preliminary analysis of random anisotropic needles systems **(P3)**

4. Marzena Jankowska (Nieradka), Teobald Kupka, Stephan P. A. Sauer, Leszek Stobiński, Noble gas probes for carbon systems **(P4)**

5. Marta Kliber, Joanna Nackiewicz, Małgorzata A. Broda, Properties of aluminium- and zinc octacarboxyphthalocyanines from the theoretical and experimental point of view **(P5)**

6. V. Zvarych; M. Stasevych; O. Dudchak; V. Poroikov; T. Gloriozova; T. Halenova, O. Savchuk, M. Vovk; V. Novikov , D. Siodłak and **T. Kupka,** Molecular modeling of structures and selected spectroscopic properties of some 1,2-derivatives of anthraquinone **(P6)**

7. Monika Ostrowska, Jacek Lipok, Paweł Kafarski**,** Interactions between cyanobacteria and metal ions - potential applications **(P7)**

8. Klaudia Radula-Janik, Teobald Kupka, Krzysztof Ejsmont, Zdzisław Daszkiewicz and Stephan P. A. Sauer, DFT studies on selected spectral parameters of carbazole derivatives **(P8)**

9. Monika Staś and Dawid Siodłak, Conformational analysis of oxazoline-L-alanine **(P9)**

10. Petr Štěpánek, Juha Vaara, Sonia Coriani, **Michal Straka**, Emerging Magneto-Optic Spectroscopy: Nuclear Spin-Induced Circular Dichroism in Fullerenes **(P10)**

11. Teobald Kupka, **Michał Stachów,** Elżbieta Chełmecka, Karol Pasterny, Magdalena Stobińska, Leszek Stobiński and Jakub Kaminský, Molecular modeling of NMR spectra for carbon nanostructures **(P11)**

12. Roksana Wałęsa, Małgorzata A. Broda, Teobald Kupka**,** DFT studies on structural and spectroscopic parameters of cytosine **(P12)**

13. V. Zvarych; M. Stasevych; O. Dudchak; V. Poroikov; T. Gloriozova; T. Halenova, O. Savchuk, M. Vovk; V. Novikov, Computer prediction, synthesis and study of protein tyrosine kinase activity of new azoles derivatives of *N*-benzoyl-*N*'-thioureas of 9,10-anthraquinone **(P13)**

14. T. Kupka, P. Tarnowski, **A. Żyła,** M. Stachów, A. Buczek, Roman Szostak, H.-M. Lin, L. Stobinski and L. -W. Fan, On the nature of pigments in red coral and African snail shell **(P14)**

15. B. Żyszka; J. Lipok, Blue green algae as potential biocatalysts for transformation of chalcones **(P15)**

IMPORTANT DATES AND DEADLINES

FINAL DEADLINES

Registration:	August 30, 2014
Payment:	August 30, 2014
Accommodation reservation:	August 30, 2014
Registration cancellation:	August 30, 2014
Submission of abstracts:	August 30, 2014
Notification of acceptance:	August 30, 2014
Submission of oral presentations:	August 30, 2014

Cancellation policy: Payments cancellations made by **August 30, 2014** entitle to a full refund less a 20% administrative fee. After that date, refund requests will not be honoured.

Notification of a cancellation must be made in writing to the Secretary via fax or e-mail.

CONFERENCE FEE*

Full-meeting participant (conference, hotel for 3 nights and meals):	650 PLN (about 160 €)
Full-meeting participant (conference fee and meals only):	350 PLN (about 90 €)
Junior scientist status (conference fee waiver, hotel for 3 nights and meals)**:	450 PLN (about 110 €)

*sum total includes 23% VAT (when applicable).
**junior scientist status (students and graduate students) must be confirmed by a letter of recommendation by a supervisor submitted together with the registration form.

The following is included in the full conference fee: conference materials, coffee breaks, lunches, dinners (and optionally 3 nights at the Villa Park Hotel).

Payment should be made to the following account:

Account holder: Restauracja Hotel Villa Park, ul. Czogały 1, 45-625 Opole, Poland

Bank name: Multibank

Account No: 57 1140 2017 0000 4802 0747 5702
SWIFT code (BIC): BREXPLPWMUL
IBAN PL: PL 57 1140 2017 0000 4802 0747 5702
Reference: mmnb2014 (Polish-Taiwanese Conference "From Molecular Modeling to nano- and biotechnology") and name of participant

Deadlines:

Payment:	August 30, 2014
Registration cancellation:	August 30, 2014

Cancellation policy: Payments cancellations made by **August 30, 2014** entitle to a full refund less a 20% administrative fee. After that date, refund requests will not be honored.

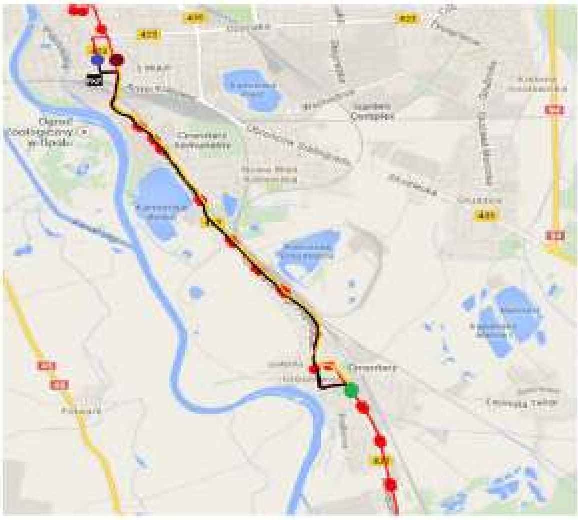
ACCOMODATION & BOARD

Accommodation at special Conference rates has been booked at Villa-Park Opole-Groszowice. This is a very well located hotel in a nice park, which provides single and double room accommodation with en suite bathrooms.

The price for one night in double room including breakfast is ca. **100 PLN or 30 € per night per person**. Total accommodation fee for three nights is included in the conference fee. Optionally, additional nights (before, or after the Conference) should be paid directly in the Hotel while leaving.

Villa-Park Opole-Groszowice address:

45-625 Opole-Groszowice, 1, Czogały Street (www.villapark.opole.pl)
Phone: +48 77 456 3508; +48 606 884 677, e-mail: hotel@ villapark.opole.pl



■ - PKP train station

● - Bus station (Kołątaja-Damrota) DEPARTURE (line 8)

● - Bus station (Oświęcimska - Szkoła) ARRIVAL and DEPARTUE (line 8)

— - route

— - return route

● - Bus station (Reymonta) ARRIVAL (line 8)

Duration : about 15 min

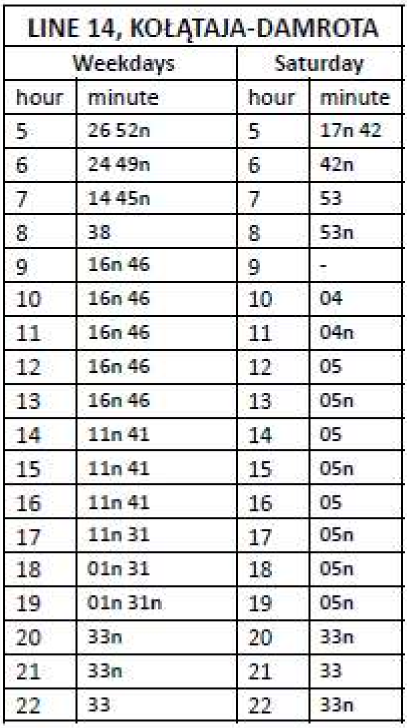
LINE 8, KOŁĄTAJA-DAMROTA			
Weekdays		Saturday	
hour	minute	hour	minute
5	30An 43n	5	38n
6	16n 47An	6	-
7	19A 36An	7	59n
8	04 31n 56An	8	-
9	-	9	54An
10	57Dn	10	-
11	57An	11	-
12	58An	12	21n
13	56An	13	-
14	15An	14	21n
15	00n 30An	15	-
16	00n	16	21n
17	44n	17	-
18	-	18	21n
19	-	19	-
20	16A	20	16An
21	15	21	-
22	15	22	15An

A - Route only to: Grotowice - Żelazna
D - Route only to Grotowice - Żelazna przez DOMECKO.
S – work days except 24 XII i 31 XII
V - work days except 24 XII
n - Low-floor vehicle

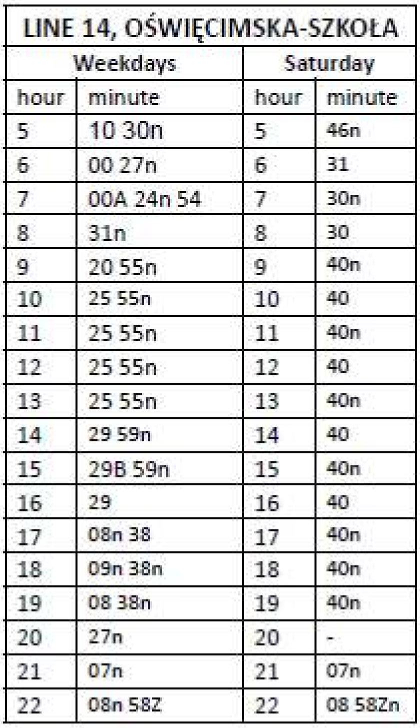
TAXI (from Opole Dworzec PKP to Villa Park); price: 30 - 35 PLN
Duration: 8 min

LINE 8, OŚWIĘCIMSKA-SZKOŁA			
Weekdays		Saturday	
hour	minute	hour	minute
5	00An 20En 40	5	05H
6	09Cn 40	6	16Cn
7	10An 18n	7	-
8	17n 55En	8	16Hn
9	-	9	-
10	09Hn	10	26Hn
11	09Hn	11	-
12	09Fn 40An	12	27Hn
13	09n 29An	13	-
14	04En 34An	14	27Gn
15	03Hn 48Cn	15	-
16	18En	16	27Gn
17	10F	17	-
18	25F	18	27Gn
19	25H	19	-
20	48F	20	23Gn
21	-	21	-
22	19Fn	22	-

A – Route only to: Polska Nowa Wieś - Centrum
C – Route: Grotowice - Dambonia - Komprachcice - Polska Nowa Wieś - Wawelno - Opole
E - Route: Grotowice - Komprachcice -Ochodze - Polska Nowa Wieś - Opole
F - Route: Grotowice - Komprachcice - Polska Nowa Wieś - Ochodze - Opole
G - Route: Grotowice - Komprachcice - Polska Nowa Wieś - Wawelno - Ochodze - Opole
H - Route: Grotowice - Komprachcice - Ochodze - Polska Nowa Wieś - Wawelno - Opole
S – work days except 24 XII i 31 XII
V - work days except 24 XII
n - Low-floor vehicle



LINE 14, KOŁĄTAJA-DAMROTA			
Weekdays		Saturday	
hour	minute	hour	minute
5	26 52n	5	17n 42
6	24 49n	6	42n
7	14 45n	7	53
8	38	8	53n
9	16n 46	9	-
10	16n 46	10	04
11	16n 46	11	04n
12	16n 46	12	05
13	16n 46	13	05n
14	11n 41	14	05
15	11n 41	15	05n
16	11n 41	16	05
17	11n 31	17	05n
18	01n 31	18	05n
19	01n 31n	19	05n
20	33n	20	33n
21	33n	21	33
22	33	22	33n



LINE 14, OŚWIĘCIMSKA-SZKOŁA			
Weekdays		Saturday	
hour	minute	hour	minute
5	10 30n	5	46n
6	00 27n	6	31
7	00A 24n 54	7	30n
8	31n	8	30
9	20 55n	9	40n
10	25 55n	10	40
11	25 55n	11	40n
12	25 55n	12	40
13	25 55n	13	40n
14	29 59n	14	40
15	29B 59n	15	40n
16	29	16	40
17	08n 38	17	40n
18	09n 38n	18	40n
19	08 38n	19	40n
20	27n	20	-
21	07n	21	07n
22	08n 58Z	22	08 58Zn

Z – Route only to: Reymonta station
n - Low-floor vehicle

Directions from the main railway station (O):

The lunches and dinners will be available at the Villa-Park Groszowice-Opole. Please mark on the registration form your request of lunch and/or dinner reservation.

CALL FOR ABSTRACTS

Plenary lecturers and authors of contributed papers (oral communications and posters) are requested to submit an abstract which will be published in the materials of the Conference. The abstracts must be prepared according to Guidelines and submitted **before August 25, 2014** to the conference secretary.

Only a limited number of oral communications can be accepted. The Scientific Committee reserves the right to accept papers. Authors will be notified about the acceptance of their contribution **before August 25, 2014**.

Oral contributions (presentations) in PowerPoint or PDF should be submitted **before August 25, 2014.**

Young Scientist Contest

We wish to encourage young scientists to attend the Conference and to present their own research on the special Young Scientists Session.

The best contributions will be awarded.

Polish-Taiwanese Conference
"From Molecular Modeling

to Nano- and Biotechnology"
Opole, 4-6 September 2014

Registration Form

Name: ***Last name:*** ***Title:***

Institution: ***Department:***

Street:

City: ***ZIP code:*** ***Country:***

Phone *(incl. country code):* ***e-mail:***

Oral communication: **yes** ☐ **no** ☐

If yes: **30 min** ☐ **15 min** ☐

Poster(s): ***yes:*** ☐ **no** ☐

Tentative title(s):

Authors:

Accommodation: ☐ **no accommodation** ☐ **Villa-Park Groszowice**

Reservation: **3/4. 09. 2014** ☐	**4/5. 09. 2014** ☐	**5/6. 09. 2014** ☐
Lunch reservation: **4.09.2014** ☐	**5.09.2014** ☐	**6.09.2014** ☐
Dinner reservation: **3.09.2014** ☐	**4.09.2014** ☐	**5.09.2014** ☐

Date:

GUIDELINES FOR ABSTRACTS AND POSTERS

We invite you all to send in your abstracts for the Conference. They will be published as a Book of Abstracts (on a CD or memory stick).

- Abstracts (1-2 pages) should be submitted by mail or e-mail as an attachment in MS Word file.
- Abstracts should be written in English, preferably in *.doc format (or *.docx).
- Abstract length: maximum 23 cm (including title, authors, authors affiliations, text and references).
- Use margins of 3.0 cm on all sides of the A4 page (21x29.7 cm).
- Font: Times New Roman, size 12, one line spacing.
- Title: CAPITAL LETTERS, on top of page, centered.
- Authors: skip one line after title. Presenting author must come first and his/her name underlined. Please give full names of all co-authors.
- Affiliations: institution, department, city and country: skip one line after authors' names.
- Text: skip one line from affiliation.
- The figures and pictures can be inserted in the abstract.

An example of abstract can be downloaded here: template

A poster stand A0 will be provided for displaying posters or alternatively several separate sheets.

CONTACT INFORMATION

All the correspondence concerning the Polish-Taiwanese Conference: "***From Molecular Modeling to Nano-and Biotechnology***"

should be directed by email

to the conference secretary(mmnb@uni.opole.pl):

M. Sc. Marzena Nieradka**, M. Sc.** Roksana Wałęsa**, M. Sc.** Aneta Buczek

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You may also contact:

Dr hab. Teobald Kupka, Prof. U. O. – chairman

teobaldk@gmail.com; teobald@uni.opole.pl

phone: +48 665 921 475

Conference Program

Wednesday, September 03, 2014	
18:00-24:00	**Registration**
Thursday, September 04, 2014	
8:00 - 9:00	**Registration**
9:00	**Opening Session**
9:15-11:15	**(S1) Session. Invited talks (*chaired* by *Szczepan Roszak*)**
9:15	**Frank Jensen** *Recent trends in force filed developments*
9:45	**Poul Erik Hansen** *Hydrogen bonding - a key modeling parameter in nano and bio-systems*
10:15	**Hong-Ming Lin** *Magnetic Hyperthermia Effects of Functionalized Iron Nanowires*
10:45	**Andrzej Bil** *Modifying The Fullerene Surface Using Endohedral Light Guests. From Ab Initio Molecular Dynamics And Metadynamics To Quantum Chemical Topology*
11:15-11:45	**Coffee break**
11:45 – 13:45	**(S2) Session. Lectures (*chaired by Frank Jensen*)**
11:45	**Michal Straka** *Endohedral Fullerenes with Actinide-Actinide Bonds: Unwilling Bonding in* $U_2@C_{80}$
12:15	**Szczepan Roszak** *Beryllium doping – the promising carbon modified materials*
12:45	**Jakub Kaminský** *Issues in modeling of Fullerenes*
13:15	**Klemens Noga** *Comprehensive support for chemistry in PL-Grid infrastructure*
13:45 – 15:00	**Lunch**
15:00 - 16:00	**(S3) Poster session:** 1. **Grzegorz Bazgier** and Jacek Lipok; Statistical computations enriching interpretation of FT-IR profiles of cyanobacteria -

metabolomic approach **(P1)**

2. **Artur Birczyński**, Grzegorz Stoch, Zdzisław T. Lalowicz, Agnieszka Szymocha Kinga Góra-Marek, Jerzy Datka;, Diverse dynamics of water molecules confined in cages of faujasites. Deuteron NMR investigation. **(P2)**
3. **D. Frączek,** R. Wiśniowski, Applying of the lattice model to a preliminary analysis of random anisotropic needles systems **(P3)**
4. **Marzena Jankowska (Nieradka),** Teobald Kupka, Stephan P. A. Sauer, Leszek Stobiński; Noble gas probes for carbon systems. **(P4)**
5. **Marta Kliber**, Joanna Nackiewicz, Małgorzata A. Broda; Properties of aluminium- and zinc octacarboxyphthalocyanines from the theoretical and experimental point of view **(P5)**
6. V. Zvarych; M. Stasevych; O. Dudchak; V. Poroikov; T. Gloriozova; T. Halenova, O. Savchuk, M. Vovk; V. Novikov, D. Siodłak and **T. Kupka**; Molecular modeling of structures and selected spectroscopic properties of some 1,2-derivatives of anthraquinone **(P6)**
7. **V. Zvarych**; M. Stasevych; O. Dudchak; V. Poroikov; T. Gloriozova; T. Halenova, O. Savchuk, M. Vovk; V. Novikov; Computer prediction, synthesis and study of protein tyrosine kinase activity of new azoles derivatives of *N*-benzoyl-*N*'-thioureas of 9,10-anthraquinone **(P7)**
8. **Monika Ostrowska**, Jacek Lipok, Paweł Kafarski; Interactions between cyanobacteria and metal ions - potential applications **(P8)**
9. **Monika Staś** and Dawid Siodłak; Conformational analysis of oxazoline-L-alanine **(P9)**
10. **Klaudia Radula-Janik**, Teobald Kupka, Krzysztof Ejsmont, Zdzisław Daszkiewicz and Stephan P. A. Sauer; DFT studies on selected spectral parameters of carbazole derivatives **(P10)**
11. Petr Štěpánek, Juha Vaara, Sonia Coriani, **Michal Straka**; Emerging Magneto-Optic Spectroscopy: Nuclear Spin-Induced Circular Dichroism in Fullerenes **(P11)**
12. Teobald Kupka**, Michał Stachów**, Elżbieta Chełmecka, Karol Pasterny, Magdalena Stobińska, Leszek Stobiński and Jakub Kaminský; Molecular modeling of NMR spectra for carbon nanostructures **(P12)**
13. **Roksana Wałęsa**, Małgorzata A. Broda, Teobald Kupka; DFT studies on structural and spectroscopic parameters of cytosine **(P13)**
14. T. Kupka, P. Tarnowski, **A. Żyła**, M. Stachów, A. Buczek, Roman Szostak, H.-M. Lin, L. Stobinski and L. -W. Fan; On the nature of pigments in red coral and African snail shell **(P14)**

	15. **B. Żyszka**; J. Lipok; Blue green algae as potential biocatalysts for transformation of chalcones **(P15)**
16:00 - 18:30	**Workshop**
18:30-20:00	**Dinner**
Friday, September 05, 2014	
9:00 - 11:00	**(S4) Session. Lectures** (c***haired by Hong-Ming Lin***).
9:00	**Tadeusz Pluta** *TDDFT determination of electric properties of excited states.*
9:30	**Yuh-Jing Chiou** *Synthesis and Characterization of Nano Hybrid MWCNTs Electrocatalysts*
10:00	**Wojciech Płonka** "Quick and dirty modeling" – importance of simplifications in computational chemistry.
10:30	**Riadh Sahnoun** *Encapsulation of hydrogen molecules inside selected fullerene cages: why the discrepancy between theoretical calculations and experimental results?*
11:00 -11:30	**Coffee break**
11.30 - 13.00	**(S5) Session. Young scientists session *(chaired by Piotr Wieczorek and Dawid Siodłak).***
11:30 11:45 12:00 12:15 12:30	**1. Monika Staś,** *Conformational properties of non-standard aminoacids with heterocyclic ring.* **2. Roksana Wałęsa, Małgorzata Broda,** *Conformational properties of compounds with N-methylated peptide bond* **3. Marzena Jankowska (Nieradka)** *Sensitivity of* ^{21}*Ne NMR parameters to nanoscopic systems* **4. Michał Stachów** *From Ethylene to plastic optical fiber*
13:00 - 14:00	Lunch

14:00 - 19:30	Guided tour to Krasiejów excavation – place of the oldest dinosaur discovery - Silesaurus opoliensis / Guided tour in Opole
19:30 - 20:30	Dinner
Saturday, September 06, 2014	
9:00 – 11:00 **9:00** **9:45**	**(S6) Session. Invited talks (*chaired by Poul Erik Hansen*).** **Tatiana Korona** *Endohedral complexes of fullerenes and other large complexes - what can we get from contemporary ab initio methods?* **Gerd Buntkowsky** *Applications of Solid State NMR on Nanocatalysts*
11: 00 - 11:30	Coffee break
11.30-13.15	Panel discussions
13.15-13.30	**Conference end**
13.30-15.00	Lunch

ABSTRACTS OF LECTURES AND POSTERS

Applications of Solid State NMR on Nanocatalysts

Gerd Buntkowsky, Torsten Gutmann, Hergen Breitzke

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In recent years, solid-state NMR spectroscopy has evolved into an important characterization tool for the study of solid catalysts and chemical processes on their surface. This interest is mainly triggered by the need of environmentally benign organic transformations. The result of this need is a large number of new catalytically active hybrid materials, which are organized on the meso- and nanoscale. Typical examples of these catalysts are supported homogeneous transition metal catalysts, transition metal nanoparticles (MNPs) or polymer based supported core shell structures. Solid-state NMR spectroscopy is able to characterize both the structures of these materials and the chemical processes on the catalytic surface. The main part of the contribution presents examples of the solid-state NMR spectroscopy characterization of Rhodium and Ruthenium containing catalysts.[1-5] Finally, first results of DNP enhanced solid state NMR spectroscopy of these systems are presented.

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Electric properties of low-lying excited states of organic molecules

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Electric properties of molecules can change significantly upon electronic excitation to excitedstates. These changes are of interst, among others, in analyzing the shift of absorption/emissionband as a function of an applied external electric field (the so-called Stark effect) e.g.[1], in attempts to understand physical basis of molecular properties in the excited states of molecules of biological interest, e.g. Retinal [2], and many others. In all these applications we need to know the value of the changes of the dipole moment and polarizability between the ground and excited states, known also as the excess dipole moment (Δμ) and excess polarizability (Δα). Despite the importance of these properties in many areas of current research our knowledge of the excited state polarizability is still rather limited.

We use the combination of widely know, well-tested TDDFT method with the finite field (FF) technique to determine the components of the excess polarizability tensor Δα. We tested our approach on a range of mid-sized organic molecules: uracil [3] diazines, p-nitroaniline and benzonitrile. We have found that the density functionals with the corrected asympotic behavior like LC-BLYP, ωB97XD and CAM-B3LYP provide more consistent and physically reliable data than standard hybrid functionals. The results of the TDDFT /FF calculations agree well with much more elaborate and expensive linear response Coupled Cluster (CCSD) calculations. Unlike the CCSD calculations our approach can be applied for the triplet state as well.

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Synthesis and Characterization of Nano Hybrid MWCNTs Electrocatalysts

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Modified Pd-based catalysts had attracted our attention because of their electrocatalytic advantages in the application of direct formic acid fuel cells (DFAFCs). To benefit the catalytic performance and prevent the catalyst poison problem, Pd based catalysts were synthesized with Au and supported on modified MWCNTs by impregnation, polyol methods and x-ray synthesis. X-ray diffraction (XRD) analysis, inductively coupled plasma-optical emission spectrometer (ICP-OES), field emission scanning electron microscopy, and high resolution electron microscopy (HRTEM) were conducted to analyze the structure, composition and morphology of the nanoparticles. The electrocatalytic performance can be measured by cyclic voltammetry (CV) in formic acid / sulfuric acid electrolyte system.

The promoting of Pd-based catalysts with Au to form solid solution and the N doped titanium oxide modified MWCNTs can significantly enhance the performance of the catalyst in formic acid electrooxidation. The newly synthesized electrocatalyst are promising for the application in direct formic acid fuel cell (DFAFCs).

Keywords: DFAFCs, palladium, gold, multi-walled carbon nanotubes, N doped titanium oxide.

Study on the Characteristics of Biogenic Calcite in *Corallium elatius*

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Abstract: *Corallium elatius*, a long-lived colonial and sessile organism, is an emblematic species of Taiwan. In spite of detailed studies, the internal structure of the axial skeleton of *Corallium elatius* is not understood. In particular, the spatial relation between the organic matrix and biogenic calcite remains in great part unexplored.

Biominerals present complex structures as a result of aggregation of crystalline “building blocks”. Fan (2007, 2013) has determined calcite in *Corallium elatius* skeleton are not pure inorganic crystals because they contain a certain amount of organic molecules which may influence polymorph selection, crystal orientation, morphology, and mechanical properties of the biominerals. In this work, the authors applies a in situ analysis which is constructed by means of sputtering ion, decalcification technique combining with SEM, TEM and EBSD on *Corallium elatius* samples As a result, the spatial distribution of sample’s organic framework is observed. Otherwise, the results of micro-examination show that different levels of “building blocks” are arranged in several hierarchies of directional modules. The modules in each hierarchical level assemble into larger units which comprise the next higher level of the hierarchy containing smaller and oriented modules. The EBSD results implied the *Corallium elatius* skeleton shows progressive transition from imperfect to perfect crystal through a hierarchical crystallographic structure.

Key words: *Corallium elatius*, biomineral, biogenic calcite

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HYDROGEN BONDING: A KEY MODELLING PARAMETER IN NANO AND BIO-SYSTEMS

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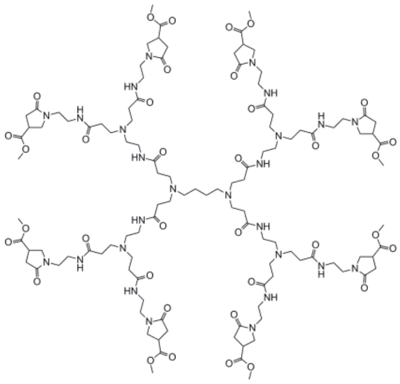
Keywords: hydrogen bonding, salt bridges, Pamam dendrimers

Hydrogen bonding is a very important parameter in the understanding structures of biological systems as well as of many nano-structures. Hydrogen is a light particle and is not so easily localized. Deuterium is better, but how large is the isotope effect? Quantum mechanical calculations clearly have a large role to play in structure determination as well as in establishing hydrogen bond potentials.

Modeling and physical constraints have to go hand in hand. The aim is to "build" simple models and understand their behavior as a function of external constrains especially charge. One of the physical constrains we have studied a lot is deuterium isotope effects on chemical shifts. This type of parameter will briefly be introduced.

The first and oldest example is that of the ammonium ion, a model for side chains of lysines and other similar cases. The models can deal both with charges and water in the solvation shell. The second model system is that of amides as fond in the backbone of proteins and peptides. An important parameter is neighboring charges. These model systems lead to discussion of salt bridges in proteins and for nan-particles to discussion of dendrimer structures.



Recent trends in force field developments

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Molecular dynamics simulations are now reaching a regime where the size of the systems and the simulation time produce results that are directly comparable to experimental results. Essentially all of these simulations rely on force field energy functions designed more than 20 years ago, and it is becoming clear that they may be the limiting component in terms of accuracy. Several initiatives aimed at introducing better energy functions for the electrostatic energy and including electronic polarization are currently in the development and testing stages. What is perhaps less known is that these approaches contain significant redundancies in the parameter space, which is computationally inefficient and potentially leads to problems in the parameterization process. After an overview of current developments in force fields, the problem of parameter redundancies will be illustrated with some recent results.

ISSUES IN MODELLING OF FULLERENES

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The nuclear magnetic resonance (NMR) spectroscopy combined with theoretical calculations is an important tool for fullerene identification. However, the accuracy of available theoretical methods is often not adequate. Therefore, we have utilized several theoretical approaches in order to address most of computational aspects needed for precise predictions of NMR properties in fullerenes.[1] The importance of the theoretical level, basis set, solvent, and molecular motions was assessed. The solvent was simulated using the implicit conductor-like polarized continuum model. The molecular motions were included via anharmonic corrections and averaging of snapshots obtained from classical and first-principles molecular dynamics (MD) simulations. Comparison to experiment revealed that density functional (DFT) calculations typically overestimate the ^{13}C NMR chemical shifts. Hybrid DFT functionals, such as BHandH and BHandHLYP, and long-range corrected functionals, such as wB97xd and CAM-B3LYP, give the best results. While the solvent has a minor effect (chemical shift changes by ~1 ppm), the vibrational and dynamical effects are surprisingly large, causing changes up to 9 ppm. Consideration of the latter was also necessary to explain the observed temperature dependence. While the dynamic corrections for MD performed in vacuum were overestimated, inclusion of the solvent in simulations provided more realistic results. The study thus points out the importance of an appropriate solvent model and a complex approach to the modelling, balancing the static, and dynamic and environmental factors.

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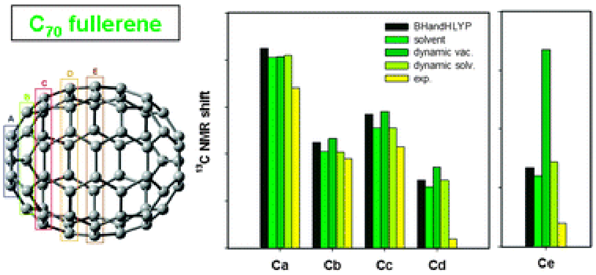

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Comprehensive support for chemistry in PL-Grid infrastructure

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PLGrid infrastructure and PLGrid PLUS, PLGrid Core and PLGrid NG projects are aimed to provide Polish researches with powerful computational infrastructure which is also tailored to the needs of specific communities. Moreover it aslo address the problem of efficient use of resources by creating domain-specific computing environments for different fields of science. In particular, domain services provide access to specialized software and support for performing common computational scenarios and multi-step experiments. Solutions and services for the community of quantum chemists are organized within the Quantum Chemistry and Molecular Physics domain.

Modern computational chemistry modelling require constantly increasing resources. More and more computational power is is needed to make larger systems (especially those being current challenges of nanotechnology or biological sciences) tractable and necessary to improve accuracy of obtained results. Fortunately, constant progress in computer technology meets this demand from scientific community. However, one must be aware that scientifically successful modelling is not just a matter of available computational resources. Equally important is the proper choice of software and efficient management of huge amount of data used in often complicated workflows. Presented projects also aim to provide tools for ease that problems. There are two kind of services for computational chemistry are under development within the Quantum Chemistry domain: InSilicoLab for Chemistry and QC Advisor.

ENDOHEDRAL COMPLEXES OF FULLERENES AND OTHER LARGE COMPLEXES- WHAT CAN WE GET FROM CONTEMPORARY AB INITIO METHODS?

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Accurate description of intermolecular interactions continues to represent a great challenge for the computational methods of quantum chemistry. The complexity of the problem is the result of a weakness of these interactions in comparison to values characteristic for chemically bonded systems, what sets stringent requirements on utilized *ab initio* methods [1]. Any supermolecular approach, selected for the calculations of intermolecular interaction energy, should properly deal with issues like size-extensivity, the basis-set superposition error, and the appropriate description of the short- and long-range electron correlation. If perturbation theory is used for intermolecular complexes, it should account for the antisymmetry properties of the supersystem wave function, as well as for the intramolecular electron-correlation effects. For both supermolecular and perturbational approaches an important issue is the utilization of sufficiently large orbital basis sets, since it turns out that the dispersion interaction, resulting from long-range correlation, saturates very slowly with the orbital basis. For post-HF methods the scaling of the computational time grows with at least fifth power of molecular size (for MP2), what makes a treatment of large molecules very (sometimes prohibitively) expensive. In the last decade, the latter problem has been partly circumvented by applying the density-fitting (DF, called also resolution-ofidentity) technique for electron-electron repulsion integrals [2]. The emergence of DF versions of HF, DFT, MP2, and SAPT methods allowed to perform calculations for much larger systems than it was possible in a not so distant past. As example applications, recent results for endohedral complexes of the C60 and C70 fullerenes with atoms and small molecules [3,4], as well as for some other intermolecular complexes, like Mg-porphyrin with various ligand molecules [5] and the nanocontainer C50H10 with CS2 [6] will be presented.

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Magnetic Hyperthermia Effects of Functionalized Iron Nanowires

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Magnetic nano materials, due to their specific physical and chemical properties, have recently been comprehensively applied to the drug delivery system, nano-bioprobe, biomarker, targeted therapy for cancer, etc. Because of these different applications, the surfaces of the materials need to have different interface designs. Therefore, when different interface materials are being synthesized, the physical and chemical stability of the magnetic nano materials, as the core of the materials, become extremely important. It is crucial that the morphology, valences, and magnetic properties of the magnetic materials need to be controlled while the functionality of modifying interfaces is synthesized on the surfaces of the magnetic nano materials.

Iron nanowires (NWs) can be fabricated via the process in which sodium borohydride reduces iron salts in external magnetic field in this study. For comparison the magnetic hyperthermia effects, iron nanowires and nanoparticles with different concentrations are heated in alternating magnetic field to measure their actual heating efficiency and SLP heating properties. The results indicate the shape effects of iron nanowires are important to enhance their heating properties. Also, the cytotoxicity of nanowires with different concentrations is measured by its survival rate in EMT-6 with the cells cultivated for 6 and 24 hours. To improve the biocompatibility of iron nanowires, the interface materials are designed in the study to modify the surface of iron nanowires (NWs), which include the SiO_2 to increase the stability of nanowires, and a modified layer of Poly(diallyldimethylammonium chloride) (PDDA) on silica to enhance the bonding of Au nanoparticles on the surface of the SiO_2/Fe NWs. This study is success to synthesize the multilayered magnetic nanowires (NWs) with biocompatible interface by means of the chemical reducing, sol-gel, chemical polymerization, and photochemical reducing. These functionalized iron nanowires including; Au/Fe NWs, Au/SiO_2/Fe NWs, and Au/PDDA/SiO_2/Fe NWs etc. The properties of these nanowires are characterized by XRD, FE-SEM, and ICP to investigate their structures, morphologies, and microchemical characteristics.

Keywords: multi-layered, functionalized, biocompatible, iron nanowire, morphologies

Beryllium doping – the promising carbon modified materials

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The controlled doping of active carbon materials leads to the enhancement of desired properties. The C/Be substitution, as the least studied, offers yet uncovered attractive possibilities. The interactions of Be_2 with Be or C atoms are dominated by large repulsive Pauli exchange contribution which balance attractive interaction terms to relatively small binding energy. The Be_2 dimer after modification due to the charge transfer and unusual intermolecular interactions constitutes the element, perpendicular to the plane of carbon network with the center of Be-Be also included in the plane. The investigation on the nature of bonding in C/Be_2 exchange complexes lead to the concept of Be_2 being the analogue of (sp^2) carbon atom and possessing the ($\sigma\pi^2$) molecular hybridization. The perturbations imposed by doped Be_2 dimers show local character regarding the structural and electronic properties of the complexes, and the separation by two carbon atoms between beryllium active centers is sufficient to consider these centers as independent sites.

UNWILLING BONDING IN $U_2@C_{80}$: ENDOHEDRAL FULLERENE WITH U-U BOND

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Abstract: The nature of bonding in previously detected[1] U_2C_{80} molecule is studied here. DFT pseudopotential calculations predict endohedral C_i $U_2@C_{80}$ with a septet ^7A_u ground state and $r_{U\text{-}U} \sim 3.9$ Å. Previous studies have shown that in small $U_2@C_{60}$ cage[2] multiple U-U bonding is forced sterically, while in larger cages, e.g., $U_2@C_{90}$,[3] the uranium atoms prefer bonding to the cage walls and U_2 unit dissociates. The $U_2@C_{80}$ system presents an interesting case in this aspect. At the minimum distance $r_{U\text{-}U} \sim 3.9$ Å the MO analysis reveals presence of two 1electron-2center bonds. The relevant MOs are formed of U(5f) orbitals. Quantum theory of atoms in molecules (QTAIM) also reveals U-U bonding. QTAIM delocalization index[4] (DI = 1.01) points to a single U-U bond (or two one-electron two-center bonds) as compared to the reference free U_2 molecule (DI = 5.98). The enclosed U atoms use their 5f electron shells to prevent unfavorable nuclear repulsion of charged U^{III}. Therefore, we coined the term "unwilling bonding" for this unique bonding pattern.

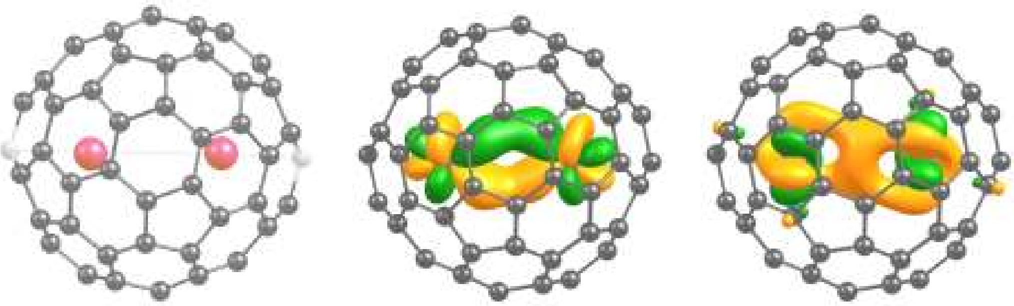

Figure 1. *The U_2C_{80} and examples of U-U 5f-5f bonding orbitals.*

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Modifying The Fullerene Surface Using Endohedral Light Guests.

From Ab Initio Molecular Dynamics And Metadynamics To Quantum Chemical Topology.

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Unlike the C_{60} molecule, C_{70} has five non-equivalent carbon atom types (commonly labelled with letters from *a* to *e*), which leads to eight non-equivalent C-C bonds. It has been shown that the *a,b*- and *c,c*- isomers are the most stable structures on the $C_{70}O$ potential energy surface, which suggests that the reaction pathway toward oxide formation must proceed via the corresponding ozonide structure. We offer a mechanism for the thermally-induced dissociation of $C_{70}O_3$. The calculations also reveal the likely time scale of the reaction (ab initio Molecular Dynamics). [1]

Although MD study gave us a clue as for the initial steps of the ozonolysis, further steps were not accessible due to the energy barrier larger than the thermal boost. Advanced technics of the free energy surface exploration, such as a metadynamics, allowed us to find structures relevant for the further steps of the reaction. The free energy surface has turned out to have complicated topology.

New achievements in the endohedral modification of fullerenes triggered questions about influence of endohedral guests on carbon atoms reactivity and properties of fullerene derivatives. We analyzed how light endohedral guests such as noble gas atoms [2], small molecules (eg. $2H_2$, H_2O, HCl, CH_4) [3] or light metal atoms [4] influence the thermodynamics of ozone ring-opening. The effect is isomer dependent, with the enthalpy of the reaction increasing for *a,b*-$C_{70}O_3$ and decreasing for *e,e*-$C_{70}O_3$ when doped with the heavy noble gas atoms Xe and Rn. In case of light molecules we observe that at room temperature the impact of the guest is small, while the electron transfer in the metal doped ozonides considerably influence the chemical property of the fullerene surface.

Quantum chemical topology provides a tool linking the concept of a chemical bond based on the Lewis theory and the quantum mechanical description of many-electron systems. We analyzed a bond evolution during the ozone ring opening on the basis of the topological features of the electron density and the electron localization function. [5]

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Sensitivity of ^{21}Ne NMR parameters to nanoscopic systems

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Abstract

Noble gas atoms (Ng) are very interesting hydrophobic probes for carbon nanosystems (see Fig. 1). These atomic probes could be monitored using nuclear magnetic resonance (NMR) techniques [1–5]. In the presented paper the potential of NMR technique in probing inner structure of porous systems including carbon nanostructures filled with inert Ng gases was analyzed theoretically. We report on accurate calculations of ^{21}Ne nuclear magnetic shieldings. The NMR parameters were calculated for a single atom, Ne dimer and a single atom encapsulated in fullerenes [6-9].

Figure 1. A single neon atom, its dimer and neon atom encapsulated inside fullerene.

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“QUICK AND DIRTY MODELING” – IMPORTANCE OF SIMPLIFICATIONS IN COMPUTATIONAL CHEMISTRY

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Applicability of computational chemistry is often hampered by expected calculation cost, which in extreme cases may exceed researcher’s lifetime and computing power available to humanity. While this may be true for modeling phenomena like protein folding, in many cases simplification of either system under investigation, or computational method may lead to useful results. Several examples will be shown ranging from polymer science to drug design.

Encapsulation of hydrogen molecules inside selected fullerene cages: why the discrepancy between theoretical calculations and experimental results?

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Abstract

Endohedral hydrogen fullerenes are chemical compounds in which one or more molecular hydrogen are encapsulated inside the fullerenes' cages. They are expected to have potential application in molecular electronics and as hydrogen carriers.

Since the synthesis of the first endohedral hydogen fullerene $H_2@C_{60}$ by Komatsu and coworkers in 2005 [1], numerous theoretical works have appeared in the literature claiming the possibility of encapsulating of as many as 29 hydrogen molecules inside C_{60} [2]. In view of the “exaggerated” number of hydrogen molecules, which not only contradicts with experimental works but also far from the experimental realization, another group of researchers have given theoretical evidence that fullerenes can accommodate only very limited number of hydrogen molecules, in line with available experimental findings.

This debate prompted us to carry out systematic investigations on selected endohedral hydrogen fullerenes in the aim of understanding the reason (or reasons) why theory “fails” to predict the “exact” number of encapsulated hydrogen molecules.

To properly describe the intermolecular interactions for this kind of endohedral complexes, dispersion or polarization interactions are likely to contribute to the intermolecular forces as much as the electrostatic ones [3]. Therefore, the method of calculation should cautiously be chosen. On the other hand, the stabilization energy, which is the criterion that determine the number of encapsulated molecular hydrogen, should be corrected for basis set superposition error (especially when larger basis sets are used) and even zero-point energy (in case when vibrational frequencies can be evaluated) [4]. Finally, the strain caused by encapsulation would involve breaking down the complex stabilization energy into guest and host molecules strain or deformation energies and host-guest interaction energy [5].

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FROM ETHYLENE TO PLASTIC OPTICAL FIBER

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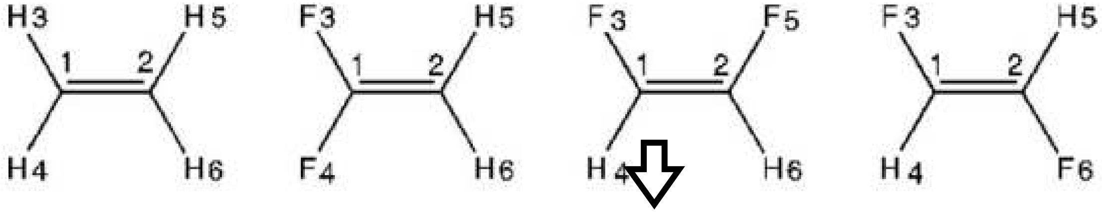
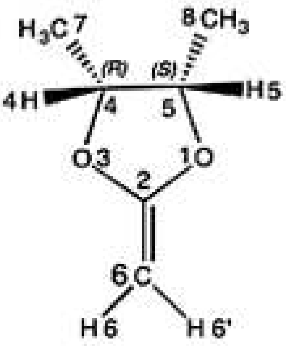
The so called “smart” materials, such as plastic optical fibers, have to meet many sophisticated requirements of modern technology. Thanks to perfluorineted polymers which are more stable, durable and resistant to corrosive environment there is a chance for progress in plastic optical fiber field.

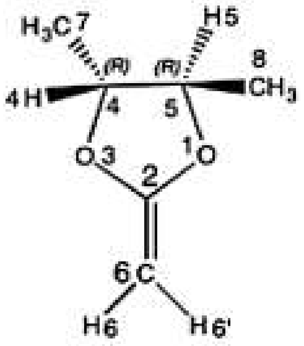
The main aim of the study was to select a theoretical methodology suitable for reliable prediction of structure, IR and Raman, as well as NMR spectra of fluorinated precursors of plastic optical fibers.

In our work we have started from the simplest model of polymer – ethylene and its perfluorinated derivatives and further on moved toward Plastic Optical Fiber (POF) precursors. We have tested several methods and basis set approaches for the best performance aimed at accurate prediction of structural and spectroscopic parameters.

The results of our studies will be presented and the best combinations of method and basis set critically discussed.







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Theoretical prediction of structural, vibrational and NMR parameters of plastic optical fiber (POF) material precursors. Cis and trans perhydro- and perfluoro-2-methylene-4,5-dimethyl-1,3-dioxolanes

J. Mol. Graphics Model. 52 (2014) 36–45.

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CONFORMATIONAL PROPERTIES OF NON-STANDARD AMINO ACIDS WITH HETEROCYCLIC RING

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Keywords: Ramachandran diagram, conformation, non-standard amino acids, heterocycles, hydrogen bond

Spatial arrangement of atoms in molecules is not accidental. The arrangement depends on intra- and intermolecular forces within molecule, for example hydrogen bond and dipole-dipole interaction. Interaction between environment and molecules is important for peptides and proteins because it can influence their conformation and thus their bioactivity. Modifications introduced into peptide main chain influence conformation by changing intra- and intermolecular interactions and cause that such modified peptides reveal specific conformational properties, and thus bioactivity. There is lack of information about conformation of non-standard amino acids residue with oxazole (Ozl), thiazole (Tzl), or oxazoline (Ozn) in place of the C-terminal amide. Some of these residues have a double bond between the carbon atoms α and β, too (Fig. 1).

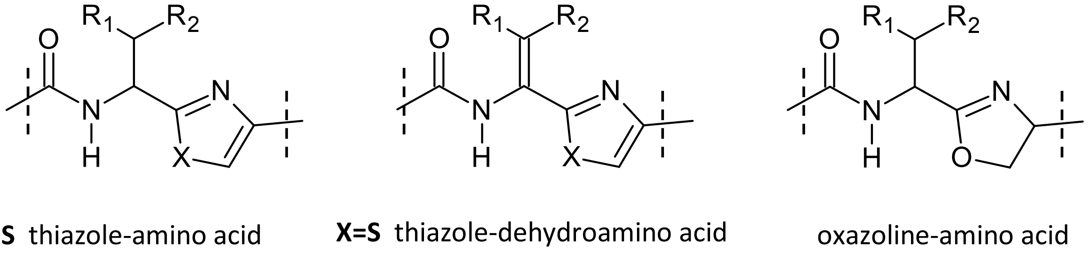

Fig. 1. Structural formula of the studied amino acid residues.

Amino acid residues with C-terminal heterocyclic ring occur in cyclic peptides like thipeptide antibiotics and alkaloids, isolated from marine organisms, fungi, and algae, which can have antitumor or antibacterial activities against bacteria Gram+ [1,2]. Series of compounds were selected to determine conformational properties of such non-standard residues: Ala-Ozl, (*Z*)-ΔAbu-Ozl, ΔAla-Ozl, Ala-Tzl, (*Z*)-ΔAbu-Tzl, ΔAla-Tzl, Ala-Ozn. Both theoretical (DFT – M06-2X) and experimental methods (IR, NMR-NOE, X-ray) were applied [3]. The obtained results indicate that a characteristic feature of the studied residues is the conformation β2. It is stabilized by N-H···N hydrogen bond formed between N-terminal amide group and the nitrogen atom of the heterocyclic ring. The conformation β2 is more stable for dehydroamino acids because of presence of π-electron conjugation and shorter N-H···N hydrogen bond. The tendency to adopt the conformation β2 decreases with increasing polarity of environment. In more polar environment the conformations β or αR are preferred. Thiazole, oxazole, and oxazoline-amino acids have rather similar conformational profile, although some differences were found.

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Conformational properties of compounds with *N*-methylated peptide bond

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The extensive studies on modifications of naturally occurring peptides are carried out to overcome their susceptibility to proteolytic degradation and to improve their permeability via biological membranes. The most common modifications are incorporation of non-coded amino acids into peptide backbone and/or *N*-methylation of amide bond. *N*-Methylation is a structural modification, in which the amide proton is replaced by *N*-methyl group (**Figure 1**).

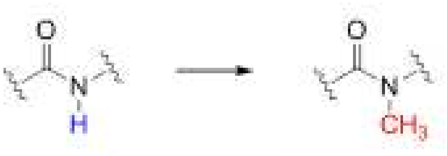

Figure 1. Secondary and tertiary amide bond.

Additional methyl groups cause steric hindrance about the *N*-methylated peptide bonds, therefore in peptides with tertiary amide bond, the reduced conformational flexibility is observed. What is more, the loss of amide's hydrogen atoms eliminates the potential formation of hydrogen bonds on the amide proton [1]. All these after-effects results in strongly dictated peptide conformation. *N*-Methylation of amide bond often provide to *cis* peptide bond conformations resulting in structures possessing completely different conformational preferences in comparison to non-methylated analogs [2]. To retain bioactive structure is essential to know the influence of tertiary amide bond on backbone conformation to enable introduction of *N*-methylated peptide bond at right position without disrupting biologically active conformation.

This work describes the conformational properties of modified amino acid residues by the example of small model diamides containing the Aib and *N*-methylglycine (peptoids) [3,4] residues. We have also investigated how *N*-methylation of the C-terminal amide bond in model dipeptides changes the conformational properties of both isomers of ⍰⍰⍰-dehydro-phenylalanine [5]. The impact of *N*-methylated peptides on the structural and dynamic properties of liposomes membranes was detected by electron paramagnetic resonance spectroscopy (ESR) enhanced by spin probes (TEMPO, 16-DOXYL) [6].

The theoretical calculations show that interactions with solvent are very important for the conformational properties of the studied diamides. The influence of water changes the number of conformers and reduces the energy difference between them. For selected peptoids the higher tendency of adopting *cis* configuration by *N*-methylated amide bond was observed, especially in aqueous environment.

We pointed out that conformational preferences of the *E* and *Z* isomers of dehydrophenylalanine residue, both with secondary and tertiary C-terminal amide bond, are distinctly different, in particular their tendency to adopt -turn conformation. Combination of ΔPhe residue with tertiary C-terminal amide bond completely change the conformational properties of the model peptides. The isomer E of the Ac-Gly-ΔPhe-NMe_2 dipeptide adopts the bend conformation easier than the isomer Z. These studies showed different impact of *N*-methylation on the main chain conformation of the neighbouring amino acid.

The ESR results showed that selected compounds with phenylalanine and -dehydrophenylalanine reduced the fluidity of liposome's membrane and the highest acitvity was observed for compound with *N*-methylated C-terminal amide bond (Ac-Phe-NMe_2). This compound, being the most hydrophobic guaranteed by additional methyl group at C-terminal amide bond, easier penetrate through biological membranes.

Acknowledgments

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Chemistry&Biodiversity – in revision

Statistical computations enriching interpretation of FT-IR profiles of cyanobacteria - metabolomic approach (P1)

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Keywords: FT-IR spectroscopy, metabolomics, cyanobacteria

Obtaining the chemical fingerprints of biological samples is one of the most interesting aspect of systematic study known as metabolomics. Among multiple applications of this methodology, not without significance is environmental metabolomics of microorganism, which allows to describe the chemical nature of interactions between microorganisms and their habitat, as well as to determine the range of response to environmental pressures.

One of the method that has proven its usefulness in obtaining the chemical profiles of microorganisms, is Fourier-Transform Infrared Spectroscopy (FT-IR). FT-IR techniques allow to obtain unique chemical-fingerprint of biota, which combine information about both the composition of particular metabolites and their chemical environment, since infrared spectra contain accurate information about crucial cellular components. Because of aggregation of the signals from each kind of intramolecular bond existing in the cells, these profiles are not easy to interpret. Therefore statistical analysis and projection of obtained results seem to play crucial role in limitation of data sets and extraction of desired information.

In our study FT-IR spectroscopy was applied to identify the differences between the strains of cyanobacteria and to trace the changes between cultures, which had grown under standard conditions and cultures suppressed by phosphonates. Observed changes exposed in some specific wavelength ranges of the spectra, were associated with important groups of cellular components. Differences in the individual spectra were recorded as changes in peaks height and position. These can be processed by statistical tools. Principle Cluster Analysis (PCA) was the major method used in our study, which allows to compare and limit the data sets. Obtained data are illustrate by statistical projection tools (dendrograms, 3D graphs), which help to find the differences and relationships between the individual samples. As a result, it can be shown which groups of cellular components of cyanobacteria are sensitive to the applied stressor. Information obtained by the aforementioned method provide valuable knowledge about the influence of phosphonates on selected aspects of metabolism of suppressed cyanobacteria.

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DIVERSE DYNAMICS OF WATER MOLECULES CONFINED IN CAGES OF FAUJASITES. DEUTERON NMR INVESTIGATION (P2)

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Keywords: deuteron quadrupole coupling, hydrogen bond, incoherent tunnelling, Pake doublet, π-jumps, water clusters, molecular dynamics, activation energy, phase transition, hysteresis

Study of dynamic behavior of water molecules in zeolites is a part of investigations aiming to elucidate also catalytic properties at molecular level. In a detailed microscopic model one expects features related to various interactions, such as electrostatic water-sodium cation, hydrogen bonding of water to framework oxygens, and water-water bonding, as well as their dependence on the loading and Si/Al ratio. There are two narrow components of different width in the spectra above 220 K for all samples considered. Their relative weights change with temperature. Contribution of the narrow component undergoes thermally activated temperature dependence and can be attributed to water molecules forming clusters freely mowing in space, with O-D performing internal tetrahedral jumps. Other water molecules perform chaotic rotational jumps, and belong to bottom adsorption layers at sodium cations. Their contribution increases on decreasing temperature. Recent relaxation measurements provide evidence for new effects. Hysteresis of spin-lattice relaxation was observed for both DY and NaY(2.4) samples at 500 % loading (280 water molecules per unit cell) in a heating-cooling cycle between 264.5 K and 277.7 K. The hysteresis is most likely reflecting formation and decomposition of water clusters at different temperature. Spin-lattice relaxation rates obtained from the experiment are consistent with a picture of the fast magnetization exchange between two dynamically different deuteron populations. The observed relaxation behaviour as a function of temperature and loading is most

likely an effect of interplay between translational and rotational diffusion. Translational diffusion of water molecules is found to be related to the strength of electrostatic interaction of water oxygen atoms to faujasite sodium cations, while water molecule reorientations seem to depend on the strength of hydrogen bonding to faujasite oxygen atoms and the strength of hydrogen bonds between water
molecules, at outer and inner positions in water clusters, respectively [1].

All molecules become localized below 220 K, as indicated by extreme broadening of the spectra, which in turn provide evidence for the symmetry of deuteron mobility. Three main components can be pointed out. Pake doublets, with the separation related to the quadrupole coupling constant, are attributed to immobile deuterons. Twofold exchange of deuteron positions leads to the characteristic spectral shape. Gaussian spectral components, with the width decreasing on increasing temperature, represent chaotic reorientations leading to narrow spectra at high temperature. Contribution of these components depends on Si/Al ratio and loading. Pake doublets dominate at temperature below 70 K, while twofold exchange was observed at the intermediate range.

A set of the quadrupole coupling constant values of localised water deuterons was derived from the analysis of the Pake dublets. Their values were attributed to deuteron positions corresponding to the locations at oxygen atoms in the faujasite framework and locations within hydrogen bonded water clusters inside faujasite cages. The contributions of the different spectral components were observed to change with increasing temperature according to the Arrhenius law with a characteristic dynamic crossover point at T = 165 K. Below T = 165 K a spectral component was observed, whose contribution changed with temperature yielding the activation energy of about 2 kJ/mol, characteristic for jumps (incoherent tunnelling) between inversion related water positions in clusters [2].

Three time constants were obtained in the spin-lattice relaxation below about 220 K. That result, common for many systems of confined molecules, can be understood as a feature reflecting a broad distribution of correlation times [3].

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Applying of the lattice model to a preliminary analysis of random anisotropic needles systems (P3)

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Keywords: Multi-scale analysis; Lattice model; Effective medium; Needles systems.

The aim of this paper is an attempt to quantitative description of random anisotropic needles systems by using ⍰$_{EMA}=f(k)$ function. In this case we use model suggested by Hattori [1] and developed by R. Piasecki, R. Wiśniowski, D. Frączek i W. Olchawa [2]. In work synthetic, computer generated patterns were examined. By computer were generate patterns at 101x101 pixels. They got changing number (from 20 to 160) randomly arranged elements at constant height (equal 2 px) and changing width (from 2 to 28 px). This patterns were researched by using rectangular sampling cells, so-called scales, with different sizes and different ⍰$_k = k_x/k_y$ (where k_x is width and k_y is sampling cells height). During numerical research were indicated universality of scales with ⍰$_k=1$. In tested range, where grouping of elements is insignificantly, confirmed that maximum k_{EMA_max} location of function ⍰$_{EMA}=f(k)$ for ⍰$_k=1$ is definitely more dependent from objects width appear in pattern than in their quantity. Examine parameter k_{EMA_max} seems to be promising determinant correlated with object width in pattern.

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DFT STUDIES ON SELECTED SPECTRAL PARAMETERS OF CARBAZOLE DERIVATIVES (P4)

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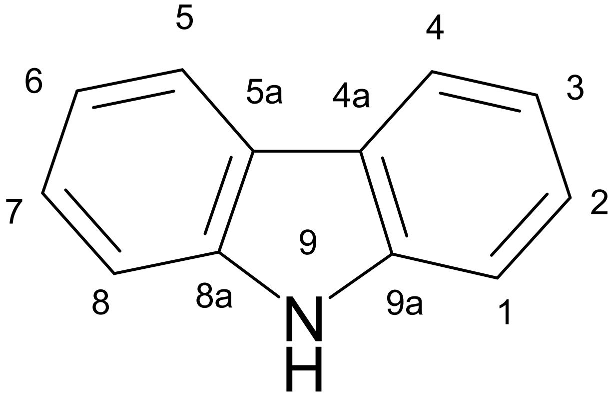
Carbazole[1–3] is an important tricyclic aromatic molecule with a central five-membered heteroaromatic ring. Formally, it is considered a derivative of fluorene with CH_2 molecular fragment replaced by NH group. Some important modifications of carbazole structure include substitution at nitrogen atom (N9) and at positions 3 and 6 of the carbazoles rings. Carbazole is characterized by high thermal stability and good photophysical properties. [4,5] Despite numerous possible applications of carbazole and its derivatives, these compounds are the most extensively studied as materials for electronics and photonics.[6-9]



In this work we report on the prediction of ^{13}C NMR chemical shifts of some carbazole derivatives. In typical theoretical works, the predicted (nonrelativistic) chemical shifts of atoms adjacent to a "heavy atom" are not accurate. This is due to the heavy atom on light atom (HALA) relativistic effects[10]. In our studies we selected the spin-orbit zeroth order regular approximation (SO ZORA) to account for the HALA effects on carbon nuclear shieldings in the dihalogeno-carbazole derivatives.

In the case of halogenated carbazoles containing several "heavy atoms" (chlorine, bromine and iodine), it was important to employ the SO ZORA approach to accurately predict and assign the observed ^{13}C NMR spectra [11, 12]. Typical nonrelativistic DFT calculations of chemical shifts of atoms C3 and C6, directly connected with the halogen atoms, produced completely meaningless results (the deviation between theory and experiment in 3,6 -diiodo-9-ethyl-9H-carbazole was about 45 ppm).

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Noble gas probes for carbon systems (P5)

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Abstract

The potential of NMR technique in probing inner structure of porous systems including carbon nanostructures filled with inert gases was analyzed theoretically. We report on accurate calculations of ^{21}Ne and ^{39}Ar nuclear magnetic shieldings. The NMR parameters were calculated for single atoms, their dimers and Ng interating with carbon systems.

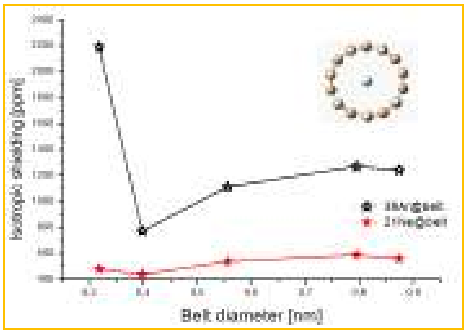

Figure 1. The sensitivity of NMR parameters of ^{21}Ne and ^{39}Ar probes encapsulated inside cyclacene belts of different diameter.

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Properties of aluminium- and zinc octacarboxyphthalocyanines from the theoretical and experimental point of view (P6)

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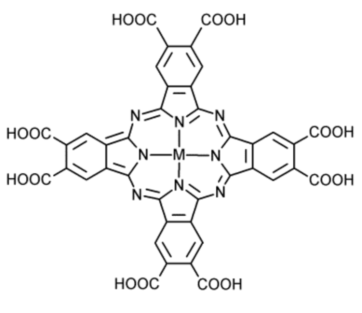
Keywords: Phthalocyanines, aluminium- and zinc octacarboxyphthalocyanine, Photodynamic therapy

Phthalocyanines (Pcs) - synthetic porphyrin analogs - are a class of macrocyclic compounds possessing a conjugated system of 18 delocalized π-electrons [1-3]. These compounds found many practical applications due to their diverse chemical, structural, electronic, and optical properties [3]. In the last decades, Pcs have been used as blue-green dyes and pigments, and also in production of liquid crystals, Langmuir–Blodgett films, gas sensors, optoelectronic devices or catalytic materials [4]. Phthalocyanines are also considered to be one of the most promising compounds in nanotechnology [5, 6]. At the present time, much attention has been focused on the possibility of using these compounds as second generation photosensitizers in photodynamic therapy (PDT) [7, 8]. The complexes of phthalocyanines with metal ions Zn^{2+} and Al^{3+}, are especially interesting in this respect because of long triplet lifetime and high triplet quantum yield. These features are essential for high singlet oxygen quantum yields and ensures high cytotoxicity against neoplasmic cells [9, 10]. Specificity in the applications of Pcs can be introduced by modification of the Pc ring or by changes in the central metal or introduction of appropriate functional groups [11].

The subject of our research are aluminium- and zinc phthalocyanines that have eight carboxylic groups attached to the benzene rings (fig. 1). The groups in aluminum 2,3,9,10,16,17,23,24-octacarboxyphthalocyanine (Al(OH)PcOC) and ZnPcOC molecules make the compounds well soluble in water. This is very important for practical applications in therapy PDT. The study of water-soluble phthalocyanines is of great theoretical and practical significance.

Fig. 1. Structure of octacarboxyphthalocyanine, M – Al(OH), Zn.



The structural and spectroscopic properties of Al(OH)PcOC and ZnPcOC will be characterized both from of theoretical as well as experimental point of view.

Acknowledgements: Marta Kliber is a recipient of a Ph.D. scholarship under a project funded by the European Social Fund.

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Molecular modeling of structures and selected spectroscopic properties of some 1,2-derivatives of anthraquinone (P7)

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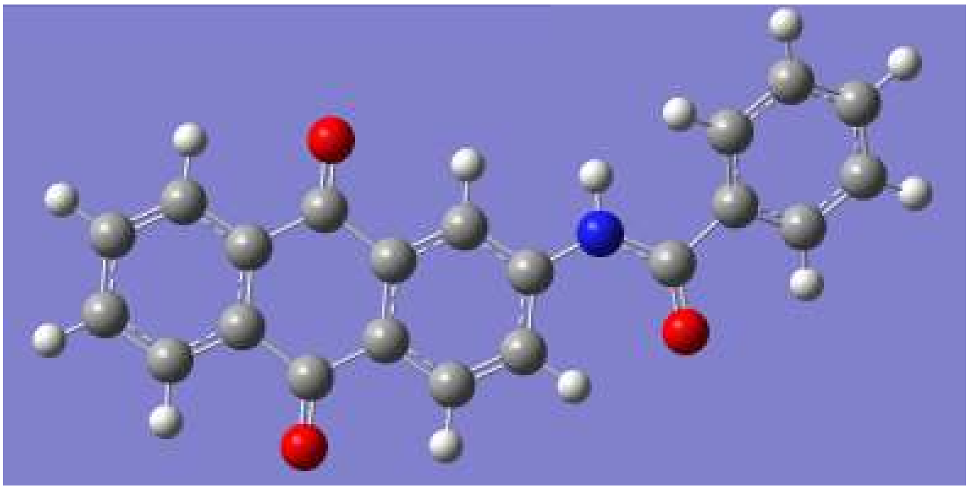
Anthraquinone derivatives have been widely used in medicine [1]. Their biological activity is closely related to their molecular and electronic structure.



In this paper we report on our preliminary molecular modeling studies of several anthraquinone derivatives using density functional theory (DFT) methodology and fairly large and flexible Pople's type basis sets.

Fully unconstrained energy minimalization was performed in vacuum at B3LYP/6-311++G(3df,2pd) level of theory. The energy minimum structures were confirmed in the subsequent vibrational studies (all harmonic frequencies were positive). Characteristic IR and Raman spectral patterns for different aromatic ring substitutions were calculated. Besides, the corresponding isotropic nuclear magnetic shieldings for the selected anthraquinones were calculated at the same level of theory. The NMR parameters were particularly sensitive to the changes in molecular structures of the studied molecules.

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INTERACTIONS BETWEEN CYANOBACTERIA AND METAL IONS - POTENTIAL APPLICATIONS (P8)

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Metallic elements are inherent component of biocenosis and occurs in the environment as a result of weathering of rocks or volcanic eruptions. But the development of industry and agriculture as well as increased range of other human activities caused contamination of environment by various forms of metals, which are especially toxic for microorganisms. Excessive accumulation of metals in ecosystems induces two type of changes in the microbial communities. At first the number of microbes is reduced, because these xenobiotics changed the activity of enzymes which participate in the process of photosynthesis, ions balance or respiration. Death of sensitive microorganisms causes the reduction of species diversity, but in the other hand it allows to grow microbes, which possess higher resistance towards certain metals.

The results of our experiments have shown that in the presence of metal ions, cyanobacteria activated various defense mechanisms, for example secretion of metabolites, which limit the direct action of metal ions toward the cells and change the chemical composition of the medium. Another observed effects were the changes in relative quantity of chlorophylls a and b, occurring in cyanobacterial cells. However the most promising, applicable effect of studied interactions was chemical transformation of metal ions into metal nanoparticles that dependent on the concentration of the ions of certain metal in culture medium, varied in morphology and intra or extracellular presence.

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This work was supported partially by Polish Ministry of Science and Higher Education in the frame of National Science Centre grant No. UMO-2011/01/B/NZ9/04722.

CONFORMATIONAL ANALYSIS OF OXAZOLINE-L-ALANINE (P9)

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Keywords: DFT, conformation, Ramachandran diagram, oxazoline, non-standard amino acid

Oxazoline-amino acids belong to non-standard amino acids. They have a unique structural modification; oxazoline ring instead of the C-terminal amide group. The oxazoline-amino acids occur in natural cyclic peptides, for example wetiellamide and bistratamide B [1]. The presence of the oxazoline ring in the main chain can influence conformational properties and thus bioactivity of peptides, however, conformational properties of such structural modification is not recognized. This research provides the conformational properties of oxazoline-L-alanine (Ala-Ozn), the simplest natural representative of this group. The studies were performed using simple model compounds: (*1S,4R/S)*-2-[1-(N-acetylamino)et-1-yl]-4-methyl-1,3-oxazoline (Fig. 1).

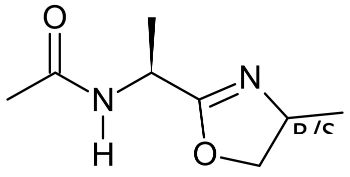

Fig.1. General formula of the studied oxazoline-L-alanine model compound, Ac-L-Ala-Ozn-4-Me.

The (φ,ψ) potential energy surfaces of Ac-L-Ala-Ozn-4-Me were calculated using the meta-hybrid M06-2X method [2]. To check the effect of environment, the presence of water and chloroform were mimicked using SMD model. Calculations show that oxazoline-L-alanine can adopt seven conformations: β2, αR, C5, β, α', αD, αL. The relative energy of the conformations change a bit in different solvents, but their number and type are constant. The energy differences between the conformations decrease with increasing polarity of the enviroment. The conformation β2 has the lowest energy in vacuo and chloroform. It is stabilized by intramolecular N-H···N hydrogen bond formed between amide group and oxazoline ring. In water environment, the lowest energy conformations are αR and β. They are stabilized by internal dipol-dipol interactions within molecule. Differences between the izomers *R* and *S* are rather small.

To confirm the results obtained, Boc-L-Ala-Ozn-COOMe model compound [3] was synthesized and presently is investigated using spectroscopic methods, FTIR and NMR, as it was performed for oxazole analogues [4].

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MOLECULAR MODELING OF NMR SPECTRA FOR CARBON NANOSTRUCTURES (P10)

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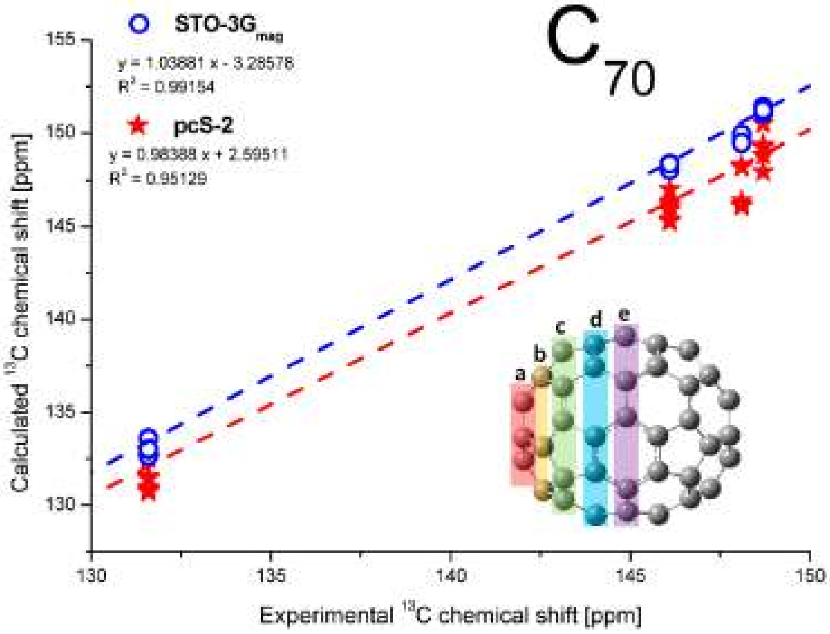
Nanoscience and nanotechnology are among those scientific fields, that are developing thanks to its commercial application potential[1, 2]. Along with that trend numerous sophisticated technical (computational) tools and solutions are developing for modeling such structures. The accuracy of predictions using *ab initio* and Density Functional Theory (DFT) levels of theory strongly depends on the design (size and completeness) of the basis set[3]. In the current work we used simple models including benzene, linear and cyclic acenes, short single wall carbon nanotube and ending with C_{60}, C_{70} and C_{76} fullerene models and STO-3G$_{mag}$ basis set, recently designed by Leszczynski and coworkers[4]. In our studies we demonstrated the applicability of STO-3G$_{mag}$ basis set for accurate prediction of selected spectroscopic properties of carbon nanosystems[5].



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Emerging Magneto-Optic Spectroscopy: Nuclear Spin-Induced Circular Dichroism in Fullerenes (P11)

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Novel magneto-optic spectroscopy techniques attract a growing interest of scientific community. The nuclear-spin optical rotation (NSOR) was observed experimentally for Xe and H2O.[1] Developments in computational methodology followed.[2]

Fresh theoretical developments have enabled the calculations of the *nuclear spin-induced circular dichroism* (NSCD),[3] a spectroscopy analogous to magnetic circular dichroism but the CD signal induced by nuclear spin magnetization instead of external magnetic field. While awaiting for the construction of efficient experimental devices we predict and analyze the first NSCD spectra for fullerenes C60 and C70.

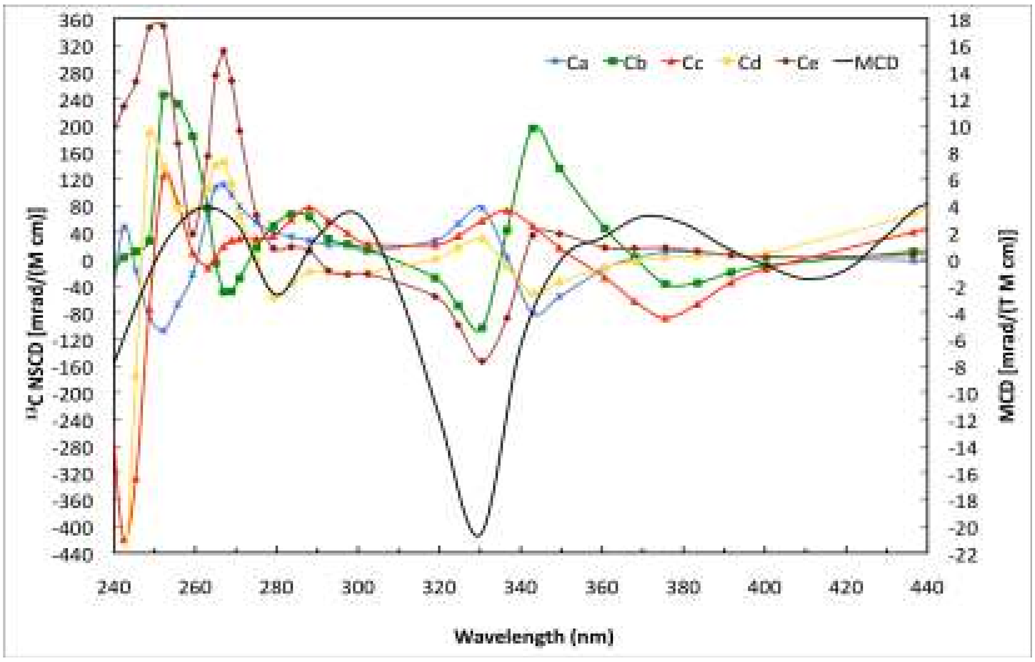

***Figure:** 13C NSCD signals for the distinct symmetry-equivalent carbon types Ca-Ce in C70.*

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DFT studies on structural and spectroscopic parameters of cytosine (P12)

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1. Introduction

From chemical point of view, cytosine is a pyrimidine derivative containing a heterocyclic aromatic ring with two substituents attached (an amine and a keto group at positions 4 and 2, respectively, **Figure 1**).

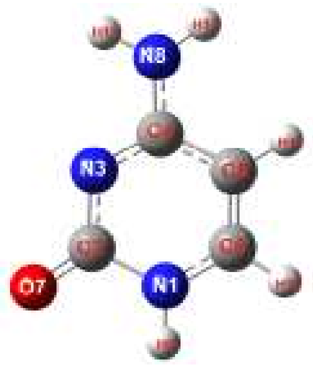

Figure 1. Chemical structure of cytosine.

Cytosine is one of the five nitrogen bases found in DNA and RNA. The formation of DNA base pairs plays a crucial role in the realization of the main role of DNA: the storage and replication of genetic information. In this context it is important to investigate the structural and spectroscopic parameters of single components of DNA base complexes [1].

The aim of the work is to study the anharmonic effects influencing structural and vibrational properties of an isolated cytosine molecule. We present here the detailed structure of cytosine in the gas phase and in DMSO solution using both harmonic and anharmonic models. In this study we also report on the extensive analysis of ^{1}H and ^{13}C nuclear magnetic shieldings at equilibrium and rovibrationally averaged structure. We also address the problem of accuracy in prediction of ^{1}H and ^{13}C NMR chemical shifts in terms of harmonic/anharmonic model, method/basis set combinations and solvent environment.

2. Methods

All calculations on keto−amino cytosine molecule were performed using Gaussian 09 software. The B3LYP method combined with 6-311++G(d,p) and 6-311++G(3df,2pd) basis sets was used to fully optimize geometry of cytosine both in the gas phase and in DMSO. The harmonic frequencies of isolated cytosine were computed at the same level of theory. The anharmonic vibration calculations were carried out in vacuo at B3LYP/6-

311++G(d,p) level of theory using the second order vibrational perturbation theory (VPT2) [2,3]. Single-point Gauge Independent Atomic Orbitals (GIAO) BHandH and B3LYP calculations of nuclear isotropic shieldings in the studied nucleobase were carried out in vacuo and in DMSO solution. Pople's 6-311++G(d,p), 6-311++G(3df,2pd), Leszczyński's STO-$3G_{mag}$ [4] and Sauer's aug-cc-pVTZ-J [5] basis sets were employed in NMR calculations. Theoretical chemical shifts were referenced to benzene calculated at the same level of theory.

3. Results

Inclusion of anharmonicity produced longer C=O bond in cytosine in the gas phase (no effect was observed in DMSO solution). The overall RMS of bond lengths in vacuum relative to experimental argon matrix results increased for R_v structure (RMS of 0.02 vs. 0.03 Å). Interaction with cytosine and solvent produced better structure (RMS of 0.01 vs. 0.015 Å for R_e and R_v models).

Theoretical wavelengths were compared with experimental data in argon matrix. The most characteristic vibrational mode (□C=O) is overestimated in the gas phase and both scaling and anharmonic treatment improves the agreement with experiment. Inclusion of solvent makes the agreement with experiment in "the gas phase" worse. The overall RMS deviations in the gas phase from experiment decrease as result of using single scaling factor or introduction of anharmonicity (RMS of 72.5, 58.1 and 50.1). A combination of anharmonicity and solvent results in worse agreement of the predicted wavelengths with experiment.

Theoretical carbon chemical shifts calculated with BHandH and B3LYP density functionals using R_e and R_v cytosine structures in vacuum and DMSO solutions are improved for rovibrationally averaged models. The introduction of solvent via polarizable continuum model (PCM) makes the agreement with experimental spectra in DMSO worse. The ^{13}C NMR data for cytosine, obtained with B3LYP are slightly better than using BHandH.

4. Acknowledgments

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Computer prediction, synthesis and study of protein tyrosine kinase activity of new azoles derivatives of

N-benzoyl-*N'*-thioureas of 9,10-anthraquinone (P13)

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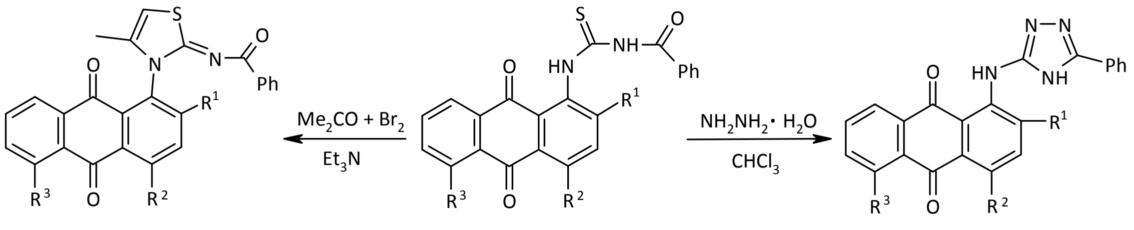
Keywords: 9,10-anthraquinones, prediction of biological activity spectra, PASS, benzoylthioureas, cyclization, thiazol-2-imines, 1,2,4-triazoles, protein tyrosine kinase activity

Many natural derivatives of the 9,10-anthraquinone and drugs based on them are widely used in medicine as an effective medications [1]. Among derivatives of aminoanthraquinone, mainly derivatives of the 1,4-diamino-9,10-anthraquinone, which containing 2-(2-hydroxyethylamino)-ethyl group at nitrogen atoms, compounds with the spectrum of pharmacological action similar to the anthracyclines and a significant antitumor activity are identified [2]. Striking examples of such aminoanthraquinones as drugs are Ametantron and Mitoxantrone. Compounds with antibacterial, antiviral, antiinflammatory [3, 4], purgative and hypoglycemic effects [1] were identified also among derivatives of 9,10-anthraquinone. In particular, the Emodyn as a derivative of 9,10-anthraquinone, has shown hypoglycemic action, antitumor activity against the lymphocytic leukemia [5], and cytotoxicity and inhibiton of precursor incorporation into DNA and RNA in HL-60 human leukemic cells [6]. It was also found, that Emodyn has inhibitory effect about protein tyrosine kinase [2, 7]. This fact has stimulated a broad search for compounds-analogues and study of their pharmacological properties to create new synthetic and semi-synthetic biologically active substances. A promising direction is to search for new low-toxic and efficient synthetic types of inhibitors of tyrosine protein kinases among derivatives of aminoanthraquinone.

The data obtained in experimental biological testing and calculated using a computer on-line program PASS [8], provided the basis for predicting probable spectrum of anticancer activity of a series of new azole derivatives of 9,10-anthraquinone [9]. Some predicted typical pharmacological effects for new anthaquinone compounds – 2-iminothiazoles **2a-e** and 1,2,4-triazoles **3a-e** [9], which include: *mucomembranous protector, transcription factor STAT3 inhibitor, antineoplastic, muramoyl-tetrapeptide carboxypeptidase inhibitor, angiogenesis inhibitor, 3-hydroxybenzoate 6-monooxygenase inhibitor, protein kinase inhibitor, pterin deaminase inhibitor, antiarthritic* etc. In the view of these calculated data using PASS the synthesis of new heterocyclic structures, including 9,10-anthraquinone, and thiazole or triazole fragments seems reasonable.

Benzoylthioureas **1a-e** were used to obtain new derivatives of 9,10-anthraquinone - N-[3-(R^1,R^2,R^3)-9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-methyl-thiazol-2(3H)-ylidene]-benzamides **2a-e** and R^1,R^2,R^3-(5-Phenyl-4*H*-1,2,4-triazol-3-yl)amino)anthracene-9,10-diones **3a-e** to search potentially antineoplastic preparations [9].



2a-e 1a-e 3a-e

$R^1=R^2=R^3=H$ (a); $R^1=Me$, $R^2=R^3=H$ (b); $R^1=R^3=H$, $R^2=NH_2$ (c); $R^1=R^2=H$, $R^3=NH_2$ (d); $R^1=R^3=H$, $R^2=NHCOPh$ (e)

Investigation of influence of anthraquinones **2** and **3** on the protein tyrosine kinase activity of membrane fractions (i.e., TPs receptor, which may be uncontrollably activated in a case of carcinogenesis) was carried out under the condition that the incubation medium with classical components and derivatives of 9,10-anthraquinone were present in concentration of 100 µM. Proteins of cell membranes of muscle tissue of nonlinear healthy rats were selected as the object of our study. The obtained results were compared, taking as 100% index of activity under the condition of presence in the incubation medium only solvent the DMSO (basal activity).

The result of investigations was established that among of the new derivatives of 9,10-anthraquinone with thiazole and triazole fragments are tyrosine kinase inhibitors of membrane-associated proteins (effect on the activity of membrane-associated tyrosine kinases within of 60-82%). These results indicate the expediency of further experimental researches with the purpose to find new potential anticancer agents in the orders of the synthesized compounds.

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On the nature of pigments in red coral and African snail shell (P14)

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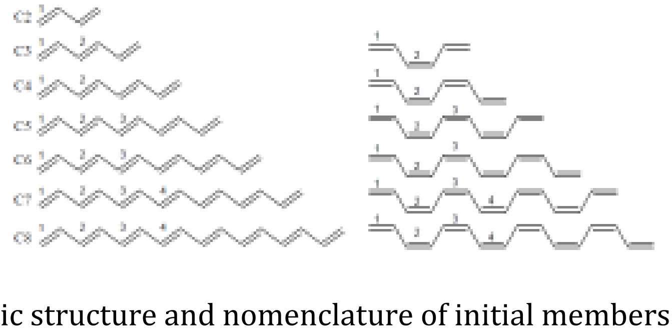
Experimental and theoretical DFT studies of red coral and African snail shell pigments are reported. B3LYP and BLYP density functionals combined with 6-31G*, 6-311++G**, pc-n and aug-pc-n basis set were used to predict the C=C harmonic stretching frequency in ethylene selected as model unit of all trans- and cis-polyenes (see Scheme 1 for structure and labeling of the studied series of compounds).

Samples of red coral (Corallium rubrum) from Taiwan and African snail (Helix Aspersa Maxima) were used in noninvasive experimental studies. The presence of all-trans polyenes containing 8 to 12 C=C units in natural pigments were confirmed by Raman spectra using 1064 laser beam and supported by theoretical modeling. In addition to typical signals due to inorganic matrix of $CaCO_3$ two Raman bands due to C=C and C-C vibrations near 1500 and 1100 cm^{-1} were observed in the studied samples.

B3LYP and BLYP modeling of structural and vibrational parameters of all-trans and all-cis polyenes using 6-311++G** basis set support the presence of 9-11 and 10-12 units C=C units in all-trans polyenes contained in pigments from red coral and African snail, respectively.



Scheme 1. Schematic structure and nomenclature of initial members of all-trans- and all-cis-polyenes

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BLUE GREEN ALGAE AS POTENTIAL BIOCATALYSTS FOR TRANSFORMATION OF CHALCONES (P15)

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Keywords: blue green algae; biotransformation; flavonoids; chalcones

Independent on the way, the obtaining of pure flavonoids whether via separation from plant material, or during chemical synthesis, is known as difficult, expensive and often requires extreme reaction conditions and toxic reagents [1]. Meanwhile the presence of flavonoids, as natural components of the cells of blue green algae (cyanobacteria) [2], suggests the biosynthesis of this substances and thereby the existence of biochemical mechanisms that enable their transformation. Cyanobacteria seem to be especially predestined for use as effective tool in structure modification of bioactive compounds to improve their physico-chemical properties, bioavailability and biological properties of maternal compounds [3]. The unique qualities of cyanobacteria such as rapid biomass increase, ease and low costs of maintaining culture, diversity of their metabolism, formation of many secondary metabolites that possessing biological activity, were just some of the reasons to commence works on interactions of cyanobacteria with chalcones. Chalcones (1,3-diarylprop-2-en-1-ones), representing flavonoids - one of the most interesting and diverse group of polyphenolic compounds, widespread in the plant kingdom, are organic compounds of a lipophilic nature, and predominantly yellow-colored. Their characteristic structural feature is 3-carbon open fragment, connecting two benzene rings. Chalcones and their derivatives, both natural and synthetic ones, possess diverse pharmacological activity [4]. The available data suggest that only heterotrophic bacteria, fungi and yeasts are able to catalyze transformations of chalcones described as: cyclizations, hydroxylations, reductions (double bonds and ketones), *O*-alkylations, dealkylations and glycosylations [5-7]. In our study, microbial transformations of chalcones were carried out using new in such activity organisms: halophilic and freshwater species of blue green algae. The influence of tested compounds on the growth of cyanobacteria was also determined. Chemical analysis of post-culture media showed the presence of newly formed substances in amount that corresponded with the disappearance of transformed chalcones. This result proves that blue green algae are able to transform chalcones what confirms the significant biotechnological potential of these microorganisms.

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