



## 2<sup>nd</sup> Polish-Taiwanese Conference

### *From Molecular Modeling to Nano- and Biotechnology*



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 2<sup>nd</sup> Polish-Taiwanese Conference:

**“From Molecular Modeling to Nano-and Biotechnology”.**

The Conference will be held in Opole, Poland from August 26 to 28, 2015 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 Conference 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, Opole, Poland*)
2. **Teobald Kupka** (*University of Opole, Opole, Poland*)
3. **Zdzisław Latajka** (*University of Wrocław, Wrocław, Poland*)
4. **Hong Ming Lin** (*Tatung Technical University, Taipei, Taiwan*)
5. **Volodymir Novikov** (*Lviv Polytechnic National University, Lvov, Ukraine*)
6. **Leszek Stobiński** (*Polish Academy of Sciences, Warsaw, Poland*)

## Organizing Committee:

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

## **Invited speakers:**

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

1. **Prof. Ko-Shao Chen** (Tatung University, Taipei, Taiwan)
2. **Prof. Yuh-Jing Chiou** (Tatung University, Taipei, Taiwan)
3. **Prof. Henryk Figiel** (AGH Kraków, Poland)
4. **Prof. Poul Erik Hansen** (Roskilde University, Denmark)
5. **Prof. Karol Jackowski** (University of Warsaw, Poland)
6. **Prof. Paweł Kafarski** (Wrocław University of Technology)
7. **Dr Jakub Kaminsky** (Czech Academy of Sciences, Prague, Czech Republic)
8. **Prof. Jacek Korchowicz** (Jagiellonian University, Krakow, Poland)
9. **Dr Tatiana Korona** (University of Warsaw, Poland)
10. **Prof. Henryk Kozłowski** (University of Wrocław, Poland)
11. **Prof. Leonid Krivdin** (Favorsky Institute of Chemistry, Irkutsk, Russia)
12. **Prof. Zdzisław Latajka** (University of Wrocław, Poland)
13. **Prof. Hong-Ming Lin** (Tatung University, Taipei, Taiwan)
14. **Prof. Volodymyr Novikov** (University of Lvov, Ukraine)
15. **Prof. Riadh Sahnoun** (University Technology Malayisa, Skudai, Malaysia)

## Plenary lectures

1. **Yun-Tsung Chang, Yuh-Jing Chiou, Hong-Ming Lin, Leszek Stobinski, Andrzej Borodzinski, Chung-Kwei Lin** *"Electrochemical Supercapacitor Behaviors Of Nano Iron Oxide/Polyaniline/Reduced Graphene Oxide Hybrid Materials"*
2. **Ko-Shao Chen, Shu-Chuan Liao, Allan Matthews, Wei-Yu Chen** *"Hybrids of Cold Plasma Process with Graft Polymers and Nano Particles for Creating Functional Surface"*
3. **Meng-Yuan Chung, Yuh-Jing Chiou, Hong-Ming Lin, Yang-Shung Lin, Andrzej Borodziński, Leszek Stobiński, Chung-Kwei Lin** *"Synthesis and Characterization of PANI-MWCNTs Supported Nano Hybrid Electrocatalysts"*
4. **Poul Erik Hansen** *"Deep Eutectic Solvents, "Anionic Liquids"*
5. **Karol Jackowski** *"Gas Phase NMR Experiments"*
6. **Paweł Kafarski** *"Inhibitors of chosen enzymes, targets for social diseases - interface of theoretical and experimental sciences"*
7. **Andrzej Kałamarz, Jan Mizera, Aneta Buczek, Teobald Kupka** *"Porous systems and water. Toward controlling water imbibition to model white hardened cement and diffusion of water and salt (NaCl) into concrete"*
8. **Jakub Kaminsky, Michał Straka** *"Efficient modelling of structural and spectroscopical parameters of nanocarbons"*
9. **Tatiana Korona** *"Intermolecular interactions and electron excitations in complexes with PCBM"*
10. **Jacek Korchowiec, A. Stachowicz-Kuśnierz, K. Liu, Y. Aoki** *"Fragmentation Techniques – a Step Towards Linear Scaling in Computational Chemistry"*
11. **Leonid Krivdin** *"Recent advances in computational NMR of the medium – sized organic molecules"*
12. **Yulia Len, Martyna Stasevych, Vira Lubenets, Natalya Marintsova, Volodymyr Novikov** *"Directions of Scientific Research activity of the Department"*
13. **Riadh Sahnoun** *"Endohedral hydrogen fullerenes: where theoretical calculations are in line with experimental results"*

## POSTERS AND LECTURES

### Lectures

1. **Mariola Czuchry, Klemens Noga, Mariusz Sterzel** „PLGrid Infrastructure. Solutions For Computational Chemistry”
2. **Lukasz Laskowski, Magdalena Laskowska, Jerzy Jelonkiewicz** "SBA-15 mesoporous silica free-standing thin films activated by copper ions - preparation and characterization”
3. **Wojciech Płonka** “Bending the iron triangle (with Moore’s law help)” – simplifications and compromises in computational chemistry”
4. **Joachim Włodarz** "PAAD: A Platform for Analysis and Archivization of Scientific Data”

### Young scientists session:

1. **Riina Aav, Silver Suun, Sven Tamp, Kerti Ausmees, Kadri Kriis, Andrus Metsala, Anna Peterson, Mario Öeren** “Assignment of configuration of chiral cyclic compounds by modelled spin-spin couplings and vibrational circular dichroism spectra”
2. **Anna Bihun, Wioletta Ochędzan-Siodłak** “Fibrous polyethylene obtained using vanadium catalysts supported on ionic liquid-modified silica”
3. **Michał Stachów, Teobald Kupka, Leszek Stobiński, Jakub Kaminsky** “Molecular modeling of SWCNTs <sup>13</sup>C NMR chemical shifts”
4. **Monika Staś, Dawid Siodłak** “Conformational properties of oxazole-amino acids and their analogues”

## Posters

1. **Anna Bihun, Aleksandra Olszowy, Wioletta Ochędzan-Siodłak** "Study of silicas modified by pyridinium ionic liquid as supports of vanadocene catalyst for ethylene polymerization"
2. **Aneta Buczek, Teobald Kupka, Małgorzata A. Broda, Katarzyna Kowalska-Szojda** "Basis set dependence of vibrational frequencies and intensities in water"
3. **Marzena Jankowska, Teobald Kupka, Leszek Stobiński** "Theoretical studies on NMR parameters of free and confined in fullerenes HD and H<sub>2</sub> molecules"
4. **Marta Kliber-Jasik, Małgorzata A. Broda, Joanna Nackiewicz** "Interactions of zinc octacarboxyphthalocyanine with selected amino acids - theoretical calculations"
5. **Tadeusz Pluta, Klaudia Radula-Janik, Teobald Kupka** "Molecular Electric Properties of Substituted Carbazole"
6. **Dawid Siodłak** " $\alpha,\beta$ -Dehydroamino acids in naturally occurring peptides"
7. **Dawid Siodłak, Monika Staś, Maciej Bujak** "Conformational differences between isomers Z and E of dehydrophenylalanine"
8. **Wioleta Śmiszek-Lindert, Elżbieta Chełmecka** "Theoretical and experimental studies on 3'-methylacetanilide (I) and 3'-methylthioacetanilide (II). Part I"
9. **Wioleta Śmiszek-Lindert, Elżbieta Chełmecka, Ewelina Kaputa-Kuc** "Theoretical and experimental studies on 4'-methylacetanilide (III) and 4'-methylthioacetanilide (IV). Part I"
10. **Roksana Wałęsa, Małgorzata Broda** "The impact of N-methylation on the  $\beta$ -turn tendency in dipeptides with Aib residue"
11. **Beata Żyszka, Emilia Kazek, Magdalena Lipok, Mateusz Zawadzki, Jacek Lipok** "Cyanobacteria as an attractive source of photosynthetic pigments and valuable bioactive natural compounds"
12. **Ryszard B. Nazarski, Lilianna Chęcińska, Magdalena Ciechańska, Andrzej Józwiak** "Hydrogen bonds in complexes of secondary amines with dimethyl sulfoxide as studied by solution NMR, DFT and aim calculations"
13. **Kornelia Czaja, Agnieszka Doskocz, Jacek Kujawski** "NMR analysis of econazole - computational calculations in chemical environment"
14. **Yang Yi, Szczepan Roszak, Jun Li** "Theoretical studies of mechanism of Traditional Chinese medicine: *Astragalus membranaceus*"
15. **Marek Doskocz, A. Rosolska, P. Durlak, P. Misiak, E. Łyczkowska-Widłak G. Banach** "E-SCIENCE.PL: specialized web-based IT platform for polish scientific laboratories. Services for scanning microscopy, NMR, crystallography labs"

## **IMPORTANT DATES AND DEADLINES**

### **FINAL DEADLINES**

Registration:	August 17, 2015
Payment:	August 17, 2015
Accommodation reservation:	August 17, 2015
Registration cancellation:	August 17, 2015
Submission of abstracts:	August 17, 2015
Notification of acceptance:	August 17, 2015
Submission of oral presentations:	August 17, 2015

Cancellation policy: Payments cancellations made by **August 17, 2015** entitle to a full refund less a 20% administrative fee. After that date, refund requests will not be honored.

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):	875 PLN (210 €)
Full-meeting participant (conference fee and meals only):	500 PLN (120 €)
Junior scientist status (conference fee waiver, hotel for 3 nights and meals)**:	775 PLN (190 €)

\* total sum 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:** mmnb2015 (Polish-Taiwanese Conference “From Molecular Modeling to nano- and biotechnology”) and name of participant

### Deadlines:

Payment: August 17, 2015

Registration cancellation: August 17, 2015

Cancellation policy: Payments cancellations made by **August 17, 2015** entitle to a full refund less a 20% administrative fee. After that date, refund requests will not be honored.

## **ACCOMODATION & BOARD**

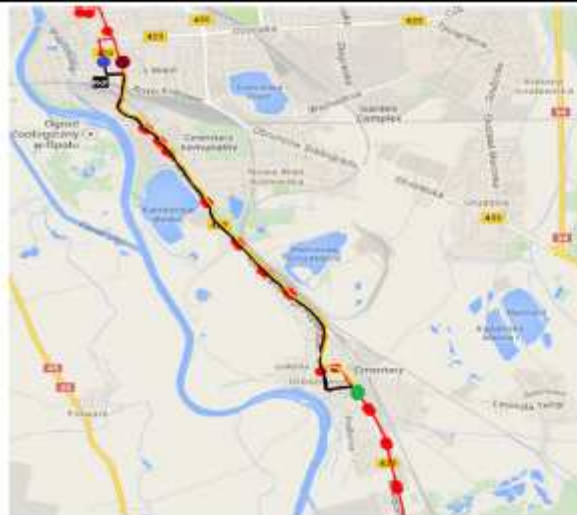
Accommodation at special Conference rates has been booked at Villa-Park Opole-Groszowice. This is a very well located hotel in a nice park, which provides single and double room accommodation with en suite bathrooms.

The price for one night in double room including breakfast is ca. 125 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](http://www.villapark.opole.pl))

Phone: +48 77 456 3508; +48 606 884 677, e-mail: [hotel@villapark.opole.pl](mailto:hotel@villapark.opole.pl)



- PKP train station
- Bus station (Kolątają-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, KOLĄTAJA-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, KOŁATAJA-DAMROTA			
Weekdays		Saturday	
hour	minute	hour	minute
5	26	5	17n 42
6	24	6	42n
7	14	7	53
8	38	8	53n
9	16n	9	-
10	16n	10	04
11	16n	11	04n
12	16n	12	05
13	16n	13	05n
14	11n	14	05
15	11n	15	05n
16	11n	16	05
17	11n	17	05n
18	01n	18	05n
19	01n	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	5	46n
6	00	6	31
7	00A	7	30n
8	31n	8	30
9	20	9	40n
10	25	10	40
11	25	11	40n
12	25	12	40
13	25	13	40n
14	29	14	40
15	29B	15	40n
16	29	16	40
17	08n	17	40n
18	09n	18	40n
19	08	19	40n
20	27n	20	-
21	07n	21	07n
22	08n	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 17, 2015** 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 17, 2015**.

Oral contributions (presentations) in PowerPoint or PDF should be submitted **before August 17, 2015**.

### **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.**



**2<sup>nd</sup> Polish-Taiwanese Conference**  
***"From Molecular Modeling to Nano- and Biotechnology"***  
**Opole, 26-28 August 2015**

**Registration Form**

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

**Institution:** **Department:**

**Street:**

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

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

<b>Oral communication:</b> yes <input type="checkbox"/> no <input type="checkbox"/> <b>If yes:</b> 30 min <input type="checkbox"/> 15 min <input type="checkbox"/>	<b>Poster(s):</b> yes: <input type="checkbox"/> no <input type="checkbox"/>
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**Tentative title(s):**

**Authors:**

**Accommodation (Villa-Park Groszowice):**     **no accommodation**

<b>Reservation:</b> 25/26. 08. 2015 <input type="checkbox"/>	26/27. 08. 2015 <input type="checkbox"/>	27/28. 08. 2015 <input type="checkbox"/>
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<b>Lunch reservation:</b> 26.08.2015 <input type="checkbox"/>	27.08.2015 <input type="checkbox"/>	28.08.2015 <input type="checkbox"/>
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<b>Dinner reservation:</b> 25.08.2015 <input type="checkbox"/>	26.08.2015 <input type="checkbox"/>	27.08.2015 <input type="checkbox"/>
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**Date and signature:**

## **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 A1 or B1 (70\*100 cm) will be provided for displaying posters or alternatively several separate sheets.

## **CONTACT INFORMATION**

All the correspondence concerning the 2<sup>nd</sup> Polish-Taiwanese Conference:  
*“From Molecular Modeling to Nano-and Biotechnology”*

should be directed by email

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

**M. Sc. Monika Staś, M. Sc. Marta Kliber, Dr Aneta Buczek**

Faculty of Chemistry  
University of Opole  
48, Oleska Street  
45-052 Opole, POLAND

### **You may also contact:**

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

[teobaldk@gmail.com](mailto:teobaldk@gmail.com); [teobald@uni.opole.pl](mailto:teobald@uni.opole.pl)

phone: +48 665 921 475



## C o n f e r e n c e   P r o g r a m

<b>Tuesday, August 25, 2015</b>	
<b>18:00-24:00</b>	<b>Registration</b>
<b>Wednesday, August 26, 2015</b>	
<b>8:00 - 9:00</b>	<b>Registration</b>
<b>9:00</b>	<b>Opening Session</b>
<b>9:15-11:15</b>	<b>(S1) Session. Invited talks (<i>chaired by prof. Paweł Kafarski</i>)</b>
9:15	<b>Yun-Tsung Chang, Yuh-Jing Chiou, <u>Hong-Ming Lin</u>, Leszek Stobinski, Andrzej Borodzinski, Chung-Kwei Lin</b> <i>"Electrochemical Supercapacitor Behaviors Of Nano Iron Oxide/Polyaniline/Reduced Graphene Oxide Hybrid Materials"</i>
9:45	<b><u>Ko-Shao Chen</u>, Shu-Chuan Liao, Wei-Yu Chen, Allan Matthews</b> <i>"Hybrids of Cold Plasma Process with Graft Polymers and Nano Particles for Creating Functional Surface"</i>
10:15	<b>Meng-Yuan chung, <u>Yuh-Jing Chiou</u>, <u>Hong-Ming Lin</u>, Yang-Shung Lin, Andrzej Borodziński, Leszek Stobiński, Chung-Kwei Lin</b> <i>"Synthesis and Characterization of PANI-MWCNTs Supported Nano Hybrid Electrocatalysts"</i>
10:45	<b>Karol Jackowski</b> <i>"Gas Phase NMR Experiments"</i>
<b>11:15-11:45</b>	<b>Coffee break</b>
<b>11:45 - 13:45</b>	<b>(S2) Session. Lectures (<i>chaired by prof. Leonid Krivdin</i>)</b>
11:45	<b>Kafarski Paweł</b> <i>"Inhibitors of chosen enzymes, targets for social diseases - interface of theoretical and experimental sciences"</i>
12:15	<b>Poul Erik Hansen</b> <i>„Deep Eutectic Solvents, "Anionic Liquids"</i>
12:45	<b>Riadh Sahnoun</b> <i>"Endohedral hydrogen fullerenes: where theoretical calculations are in line with experimental results"</i>
13:15	<b>Yulia Len, Martyna Stasevych, Vira Lubenets, Natalya Marintsova, <u>Volodymyr Novikov</u></b> <i>"Directions of Scientific Research activity of the Department"</i>
<b>14:00 - 15:00</b>	<b>Lunch</b>
<b>15:00 - 16:00</b>	<b>(S3) Poster session:</b>
	<b>1. <u>Anna Bihun</u>, Aleksandra Olszowy, Wioletta Ochędzan-Siodłak</b> <i>"Study of silicas modified by pyridinium ionic liquid as"</i>

- supports of vanadocene catalyst for ethylene polymerization”
2. **Aneta Buczek, Teobald Kupka, Małgorzata A. Broda, Katarzyna Kowalska-Szojda** *“Basis set dependence of vibrational frequencies and intensities in water”*
  3. **Kornelia Czaja, Agnieszka Doskocz, Jacek Kujański** *“NMR analysis of econazole - computational calculations in chemical environment”*
  4. **Marek Doskocz, A. Rosolska, P. Durlak, P. Misiak, E. Łyczkowska-Widłak G. Banach** *“E-SCIENCE.PL: specialized web-based IT platform for polish scientific laboratories. Services for scanning microscopy, NMR, crystallography labs”*
  5. **Marzena Jankowska, Teobald Kupka, Leszek Stobiński** *“Theoretical studies on NMR parameters of free and confined in fullerenes HD and H<sub>2</sub> molecules”*
  6. **Marta Kliber-Jasik, Małgorzata A. Broda, Joanna Nackiewicz** *“Interactions of zinc octacarboxyphthalocyanine with selected amino acids - theoretical calculations”*
  7. **Ryszard B. Nazarski, Lilianna Chęcińska, Magdalena Ciechańska, Andrzej Józwiak** *“Hydrogen bonds in complexes of secondary amines with dimethyl sulfoxide as studied by solution NMR, DFT and aim calculations”*
  8. **Klaudia Radula-Janik, Tadeusz Pluta, Teobald Kupka** *“Molecular Electric Properties of Substituted Carbazole”*
  9. **Dawid Siodłak** *“ $\alpha,\beta$ -Dehydroamino acids in naturally occurring peptides”*
  10. **Dawid Siodłak, Monika Staś, Maciej Bujak** *“Conformations differences between isomers Z and E of dehydrophenylalanine”*
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  13. **Roksana Wałęsa, Małgorzata Broda** *“The impact of N-methylation on the  $\beta$ -turn tendency in dipeptides with Aib residue”*
  14. **Yang Yi, Szczepan Roszak, Jun Li** *“Theoretical studies of mechanism of Traditional Chinese medicine: Astragalus membranaceus”*
  15. **Beata Żyszka, Emilia Kazek, Magdalena Lipok, Mateusz Zawadzki, Jacek Lipok** *“Cyanobacteria as an attractive source of photosynthetic pigments and valuable bioactive natural compounds”*

16:00 - 18:30

Workshop

18:30-20:00

Dinner

**Thursday, August 27, 2015**

<b>9:00 - 11:15</b>	<b>(S4) Session. Lectures (chaired by prof. Małgorzata Broda / prof. Zofia Drzazga)</b>
9:00	<b><u>Jakub Kaminsky, Michał Straka</u></b> "Efficient modelling of structural and spectroscopical parameters of nanocarbons"
9:30	<b>Andrzej Kałamarz, Jan Mizera, Aneta Buczek, Teobald Kupka</b> "Porous systems and water. Toward controlling water imbibition to model white hardened cement and diffusion of water and salt (NaCl) into concrete"
9:45	<b>Joachim Włodarz</b> "PAAD: A Platform for Analysis and Archivization of Scientific Data"
10:00	<b><u>Lukasz Laskowski, Magdalena Laskowska, Jerzy Jelonkiewicz</u></b> "SBA-15 mesoporous silica free-standing thin films activated by copper ions - preparation and characterization"
10:15	<b>Mariola Czuchry, <u>Klemens Noga</u>, Mariusz Sterzel</b> „PLGrid Infrastructure. Solutions For Computational Chemistry”
10:45	<b>Wojciech Płonka</b> "Bending the iron triangle (with Moore's law help)" – simplifications and compromises in computational chemistry"

**11:15 -11:45** Coffee break

<b>11:45 - 13:00</b>	<b>(S5) Session. Young scientists session (chaired by dr Dawid Siodłak).</b>
11:45	<b><u>Riina Aav, Silver Suun, Sven Tamp, Kerti Ausmees, Kadri Kriis, Andrus Metsala, Anna Peterson, Mario Öeren</u></b> "Assignment of configuration of chiral cyclic compounds by modelled spin-spin couplings and vibrational circular dichroism spectra"
12:00	<b><u>Anna Bihun, Wioletta Ochędzan-Siodłak</u></b> "Fibrous polyethylene obtained using vanadium catalysts supported on ionic liquid-modified silica"
12:15	<b><u>Michał Stachów, Teobald Kupka, Leszek Stobiński, Jakub Kaminsky</u></b> "Molecular modeling of SWCNTs <sup>13</sup> C NMR chemical shifts"
12:30	<b><u>Monika Staś, Dawid Siodłak</u></b> "Conformational properties of oxazole-amino acids and their analogues"

**13:00 - 14:00** Lunch

14:00 - 17:30	Guided tour in Opole – <b>Open air ethnographic museum of Opole village</b>
18:30 - 20:30	Dinner
<b>Friday, August 28, 2015</b>	
9:00 – 11:00	<b>(S6) Session. Invited talks (chaired by prof. Poul Erik Hansen).</b>
9:00	<b>Leonid Krivdin</b> <i>“Recent advances in computational NMR of the medium – sized organic molecules”</i>
9:45	<b>Tatiana Korona</b> <i>“Intermolecular interactions and electron excitations in complexes with PCBM”</i>
10:30	<b>Jacek Korchowiec, A. Stachowicz-Kuśnierz, K. Liu, Y. Aoki</b> <i>“Fragmentation Techniques – a Step Towards Linear Scaling in Computational Chemistry”</i>
11:00 - 11:30	Coffee break
11:30-13:15	Panel discussions
<b>13:15-13:30</b>	<b>Conference end</b>
13:30-15:00	Lunch



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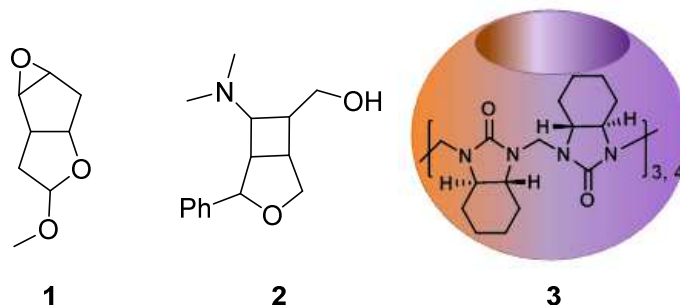
# Assignment of configuration of chiral cyclic compounds by modelled spin-spin couplings and vibrational circular dichroism spectra

Riina Aav, Silver Suun, Sven Tamp, Kerti Ausmees, Kadri Kriis, Andrus Metsala, Anna Peterson, Mario Öeren

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**Keywords:** chiral compounds, macrocycles, NMR, VCD, DFT

Determination of relative configuration of substituents in a 5-membered ring by NMR spectroscopy is a complicated task, due to the possibility of several energetically close conformations. Therefore modelling studies were coupled with assignment of NMR spectra. We have shown, that quantum chemical approach for assignment of relative configuration by  $^3J(H,H)$  coupling constant of bicyclo[3.3.0]octanes **1** is highly reliable.<sup>1</sup> In this presentation applicability of  $^3J(C,H)$  and  $^2J(C,H)$  coupling constants and assignment of relative configuration of bicyclo[3.2.0]heptanes **2** will be shown. In addition to relative configuration, also determination of absolute configuration of chiral compounds is of great importance. NMR method itself does not discriminate enantiomers, hence the vibrational circular dichroism (VCD) is the method of choice for the analysis of solutions. We will report that chiral hemicucurbiturils<sup>2,3</sup> **3** have specific VCD signals of urea functional groups, which reflects the orientation of monomers. The assignment of VCD signals demands modelling, and problems associated with it will be discussed.



**Fig. 1.** Structures of bicyclo[3.3.0]octanes **1**, bicyclo[3.2.0]heptanes **2** and cyclohexylhemicucurbit[6,8]urils **3**

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# STUDY OF SILICAS MODIFIED BY PYRIDINIUM IONIC LIQUID AS SUPPORTS OF VANADOCENE CATALYST FOR ETHYLENE POLYMERIZATION

Anna Bihun; Aleksandra Olszowy; Wioletta Ochędzan-Siodłak

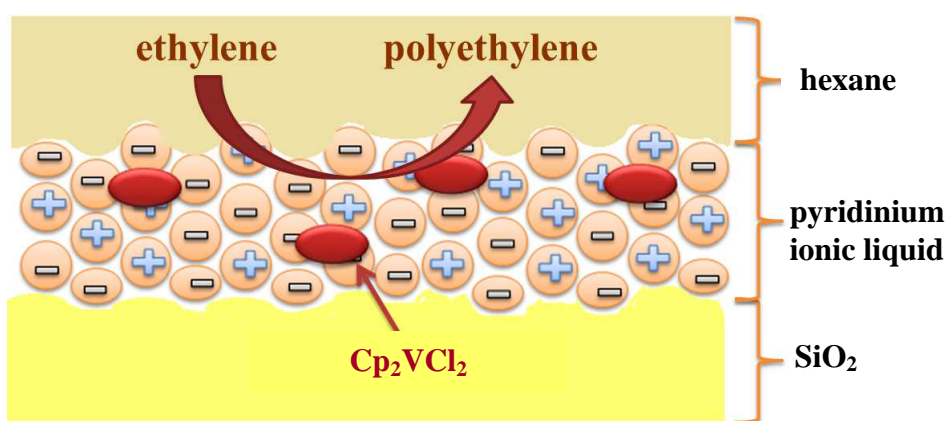
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**Keywords:** ethylene polymerization, vanadocene catalyst, pyridinium ionic liquid, silica support

Heterogenization of catalysts for coordination  $\alpha$ -olefin polymerization on a solid support is important method to control of polymer morphology. Silica is the most often used, because of its low cost, non-toxicity, ability to obtain various size and morphology of the support particles with large surface area. Silica is characterized by considerable stability, both physical and chemical, and on the other hand, it is possible to modify its structure: chemically, thermally or mechanically. "Chemistry of surface" of the silica is not only relatively simple, but also universal, which enables heterogenization of catalytic systems using various methods [1].

One of new methods for heterogenization of organometallic catalysts is Supported Ionic Liquid (SIL) strategy, in which a catalyst is dissolved in a thin layer of an ionic liquid immobilized on a solid, porous support (e.g.  $\text{SiO}_2$ ,  $\text{TiO}_2$ ,  $\text{Al}_2\text{O}_3$  etc.). Very important advantage of this type of catalysts is a possibility to be tuned by changing the solid support, ionic liquid and catalyst [2-5].

In our investigations, a series of SIL systems with the  $\text{Cp}_2\text{VCl}_2$  vanadocene catalyst was synthesized by immobilization of the pyridinium ionic liquid on various types of silica, which differ in surface areas and pore sizes (Fig. 1).



**Fig. 1.** SIL system for ethylene polymerization

We have also synthesized, as reference systems, heterogeneous vanadocene catalysts without the ionic liquid. The prepared systems were analyzed by FTIR, elemental analysis, BET, AAS, and SEM methods. We checked the influence of the ionic liquid and the type of silica on the performance of the ethylene polymerization and



of the polymer properties. It turned out that all studied catalyst systems were active in the ethylene polymerization, regardless of the type and amount of alkylaluminum activator (AlEtCl<sub>2</sub> or AlEt<sub>2</sub>Cl). The best results, it means the highest activity, was obtained using the SIL system with the silica having regular morphology, modified by the pyridinium chloroaluminate ionic liquid, and the AlEtCl<sub>2</sub> activator. All synthesized catalytic systems allow to receive linear PE with high average molecular weight ( $M_w > 1 \cdot 10^6$  g/mol) and narrow molecular weight distribution ( $1.5 < M_w/M_n < 3.7$ ), regardless of the type of silica, composition of the catalytic system and the polyreaction conditions. Application of the silica supports without ionic liquid results in PE granules, which reflects the support morphology, whereas the polymer obtained using the studied SIL systems has an unusual, fibrous structure.

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# FIBROUS POLYETHYLENE OBTAINED USING VANADIUM CATALYSTS SUPPORTED ON IONIC LIQUID-MODIFIED SILICA

Anna Bihun; Wioletta Ochędzan-Siodłak

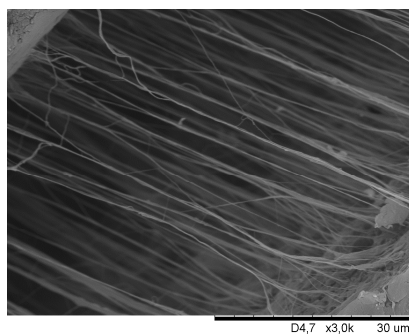
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**Keywords:** polyethylene, vanadium catalysts, imidazolium ionic liquid, silica

The vanadium catalysts immobilized on a solid carrier, e.g. magnesium chloride or silica, produce polyethylene characterized by high molecular weight, but broad molecular weight distribution [1, 2]. Polyethylene, especially high molecular weight polyethylene, is an attractive product because of its good physical and mechanical properties. Nevertheless, the presence of long and entangled polymer chains makes a considerable difficulty in processing. This can be changed by obtaining the polymer in form of fibres. Polyethylene fibres can be obtained in post-reactor method by crystallization from solution or by melt-drawing [3]. Another way is to obtain fibrous polyethylene directly from reactor during polymerization, through a suitable choice of both catalyst and reaction parameters.

Heterogeneous metallocene catalysts for coordination ethylene polymerization, due to the presence a solid support, enable to control the polymer morphology [4-6]. Selection of both support and method of immobilization has a great influence, not only on properties of the resulting polymer, but also on the polymerization performance [6]. Direct synthesis of the fibrous polyethylene having improved properties is attractive for industry, thus it deserves further investigation [3]. In recent years, the supported-ionic liquid (SIL) strategy became promising method of heterogenization of organometallic catalysts for olefin polymerization and oligomerization. In this method the thin layer of an ionic liquid (IL), which contains dissolved catalyst, is immobilized on a solid support (e.g. SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub> etc.) [8, 9]. The SIL system can be tuned by optimizing structures of the ionic liquid, transition-metal catalyst, and solid support [9-11].

We applied the SIL strategy for heterogenization of metallocene and post-metallocene vanadium catalysts. The SIL systems consisted of the silica solid support covered by thin film of the 1-(3-triethoxysilyl)propyl-3-methylimidazolium chloroaluminate ionic liquid, in which the Cp<sub>2</sub>VCl<sub>2</sub> or VCl<sub>2</sub>(salenCl<sub>2</sub>) precursor were placed. Such prepared vanadium catalysts, after activation by AlEtCl<sub>2</sub> or AlEtCl<sub>2</sub>, were applied in ethylene polymerization. The result is an unusual polyethylene with fibrous morphology (Fig. 1), high molar weight appropriate for vanadium heterogeneous catalysts [1, 2] and narrow molecular weight distribution typical for homogeneous metallocene and postmetallocene catalysts [12].



**Fig. 1.** SEM image of fibrous PE

The polymer was characterized by FTIR,  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, DSC, GPC, SEM and WAXS methods. The SIL systems reveal higher activity (up to 2 tons PE(molV·h) $^{-1}$ ) and stability during reactions than homogeneous analogues.

The studies show the method of obtaining fibrous polyethylene in direct synthesis using vanadium catalysts supported on the SIL system. The fibrous morphology of the obtained polyethylene results basically from the applied catalyst precursors and the kind of the activator as well as reaction parameters. It should be noted that the obtained fibrous polyethylene has high molecular weight, typical for the supported catalyst, and narrow molecular weight distribution, characteristic for the homogeneous metallocene and post-metallocene catalysts. This specific junction of both features seems to be connected with the applied SIL strategy.

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# BASIS SET DEPENDENCE OF VIBRATIONAL FREQUENCIES AND INTENSITIES IN WATER

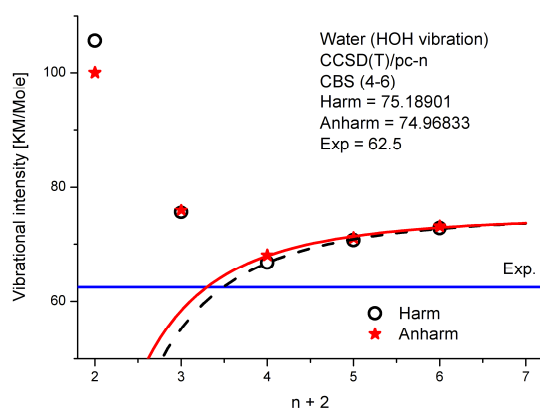
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Basic molecular modeling of structure and spectroscopic parameters relies on unconstrained geometry optimization followed by frequency calculations. With the improvement in the method of calculation and one electron basis set one hopes to reproduce experimental parameters more accurately. However, theory is able to predict very accurate geometric parameters while vibrational frequencies are more difficult. The intensities of vibrational bands are very important for correct assignment of IR/Raman. These parameters are far more difficult to predict theoretically than frequencies.

Water was selected as a small model molecule to test the convergence of vibrational frequencies and intensities of  $\nu_{\text{OH}}(\text{sym})$ ,  $\nu_{\text{OH}}(\text{asym})$ ,  $\delta_{\text{HOH}}$  modes using several theoretical methods and families of regularly converging Dunning and Jensen type basis sets. Some results were estimated in the complete basis set limit (CBS) using a popular two-parameter formula. In this paper we will discuss the performance of several methods combined with specific basis sets and propose some hints leading to accurate calculation of water vibrational intensities.



**Figure 1** Convergence of HOH band intensity toward CBS (CCSD(T)/pc-n, where  $n = 0 - 4$ , lines are obtained from two-parameter fitting using three last data points)

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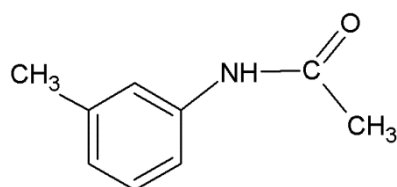
# THEORETICAL AND EXPERIMENTAL STUDIES ON 3'-METHYLACETANILIDE (A) AND 3'-METHYLTHIOACETANILIDE (B). PART I

Wioleta Śmiszek-Lindert<sup>1</sup>, Elżbieta Chelmecka<sup>2</sup>

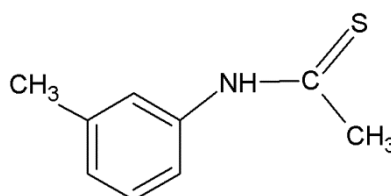
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The X-ray structure, theoretical calculation, Hirshfeld surfaces analysis, IR spectra of 3'-methylacetanilide and 3'-methylthioacetanilide were reported.



**3'-metyloacetanilide**  
(A)



**3'-methyltioacetanilide**  
(B)

Theoretical calculations of the title compounds isolated molecule have been carried out using DFT at the B3LYP/6-311++G(3df,2pd) level. The intermolecular interactions in the crystal structure, for both compounds, were analyzed using Hirshfeld surfaces computational method (Fig. 1 (a) and (b), as well as Fig. 2 (a) and (b)). The Hirshfeld surface analyses were carried out using the CrystalExplorer program. Distance from the Hirshfeld surface to the nearest nucleus inside and outside the surface has been marked by  $d_i$  and  $d_e$ , respectively. Whereas,  $d_{norm}$  is a normalized contact distance, which has been defined in turn of  $d_i$ ,  $d_e$  and the van der Waals (vdW) radii of the atoms [1]:

$$d_{norm} = \frac{d_i - r_i^{vdW}}{r_i^{vdW}} + \frac{d_e - r_e^{vdW}}{r_e^{vdW}}$$

$d_{norm}$  has been visualized using a red-white-blue colour scheme. If the atoms make intermolecular contacts closer than the sum of their vdW radii, these contacts will be represented as red spots on the surface. Longer contacts are blue, and white colour is used for contacts around the sum of van der Waals radii. Hirshfeld surface analysis was used for visually analyzing intermolecular interactions in the crystal structure of 3'-methylacetanilide and 3'-methylthioacetanilide.

The details of our research will be presented and discussed.

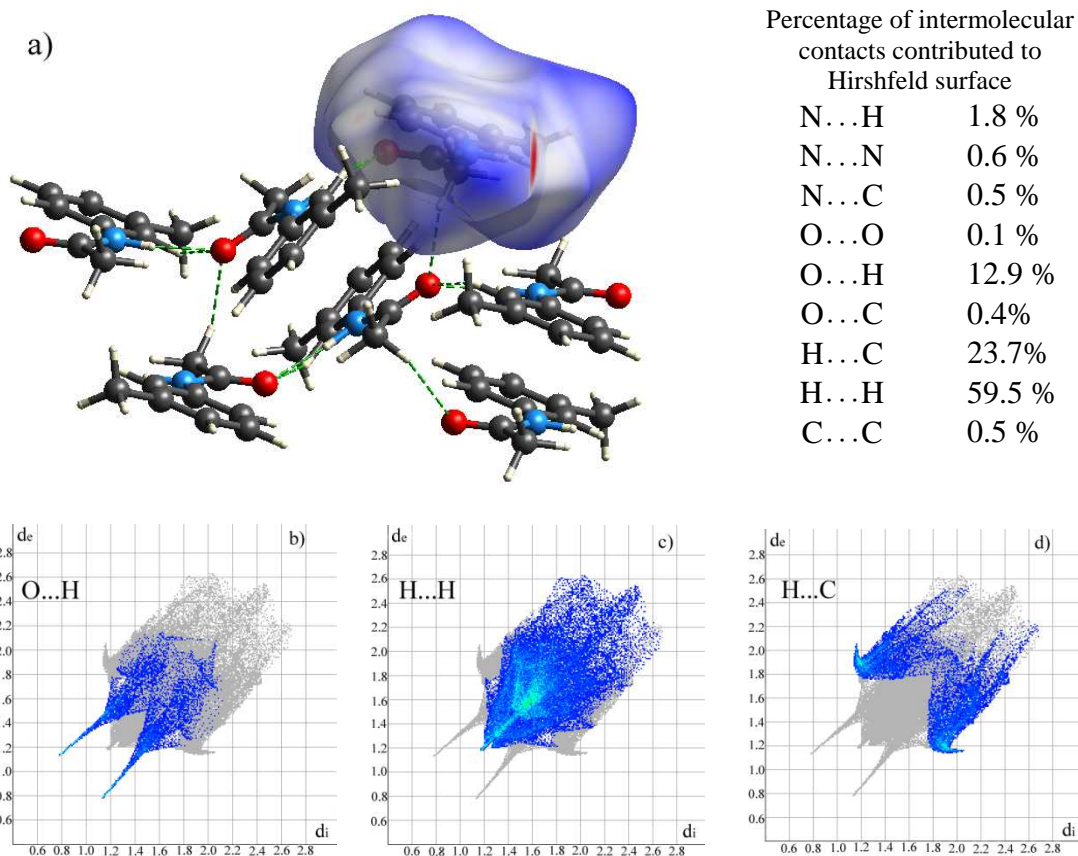
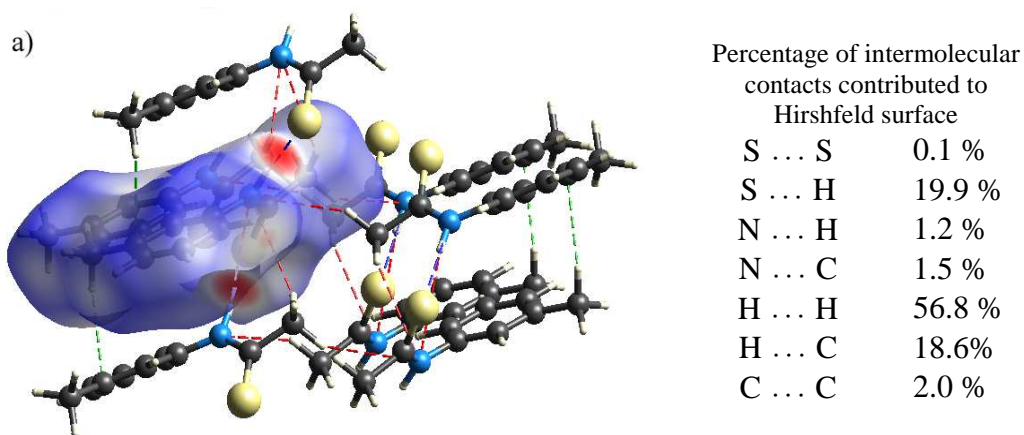


Fig. 1. Hirshfeld surface; a)  $d_{norm}$  mapped on Hirshfeld surface for visualizing the intercontacts of the 3-methylacetanilide. Dotted lines represent hydrogen bonds; b); c); d) fingerprint of the 3-methylacetanilide.  $d_i$  is the closest internal distance from a given point on the Hirshfeld surface and  $d_e$  is the closest external contacts.



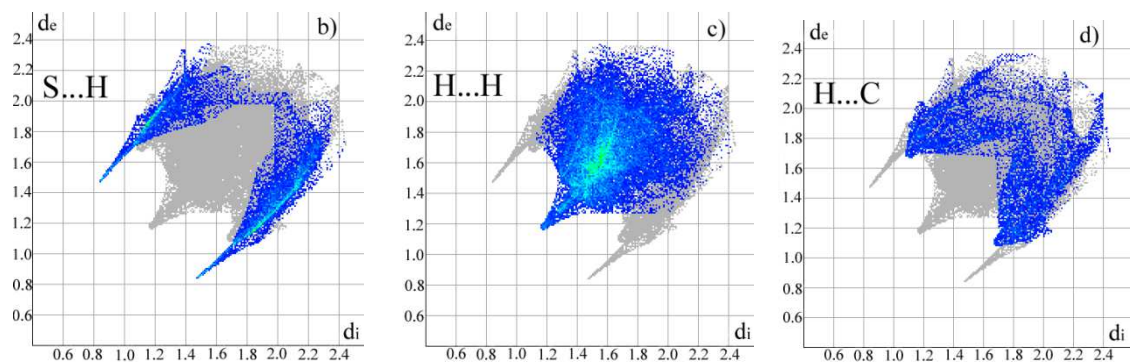


Fig. 2. Hirshfeld surface; a)  $d_{norm}$  mapped on Hirshfeld surface for visualizing the intercontacts of the 3'-methylthioacetanilide. Dotted lines represent hydrogen bonds; b); c); d) fingerprint of the 3'-methylthioacetanilide.  $d_i$  is the closest internal distance from a given point on the Hirshfeld surface and  $d_e$  is the closest external contacts.

### Acknowledgement

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All of the calculations were performed with the aid of hardware and software at the Wrocław Centre for Networking and Supercomputing WCSS, Wrocław, Poland.

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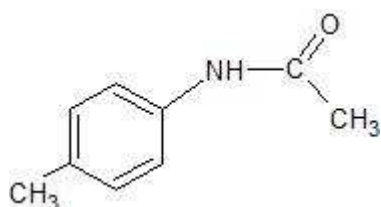
# THEORETICAL AND EXPERIMENTAL STUDIES ON 4'-METHYLACETANILIDE (C) AND 4'-METHYLTHIOACETANILIDE (D). PART II

Wioleta Śmiszek-Lindert<sup>1</sup>, Elżbieta Chełmecka<sup>2</sup>, Ewelina Kaputa-Kuc<sup>1</sup>

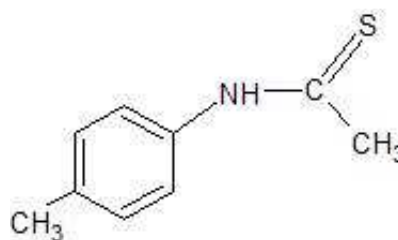
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In this work we analyze the relation between molecular structure of amides and thioamides. The X-ray structure, theoretical calculation and Hirshfeld surfaces analysis of 4'-methylacetanilide and 4'-methylthioacetanilide were reported.



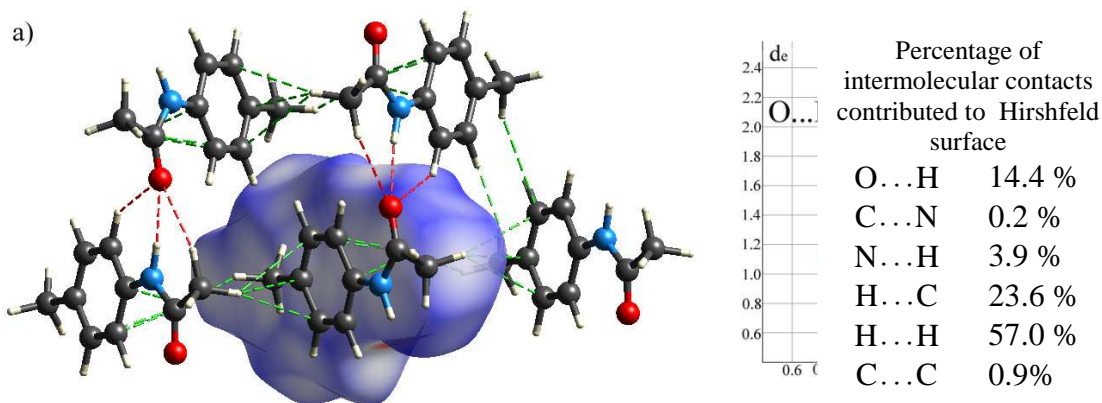
**4'-metyloacetanilide  
(C)**



**4'-metyloacetanilide  
(D)**

The molecules of A and C, as well as B and D are connected by C-H...O and C-H...S hydrogen bonds respectively. The strength of the hydrogen bond was also confirmed by IR spectroscopy. The structure of the experimental IR spectrum has been correctly reproduced by B3LYP/6-311++G(3df,2pd) calculations. The intermolecular interactions in the crystal structure, for both compounds, were analyzed using Hirshfeld surfaces computational method (see Fig. 1 (a) - (e), and Fig. 2 (a) - (d).

The significance differences between structures all compounds will be presented and discussed.





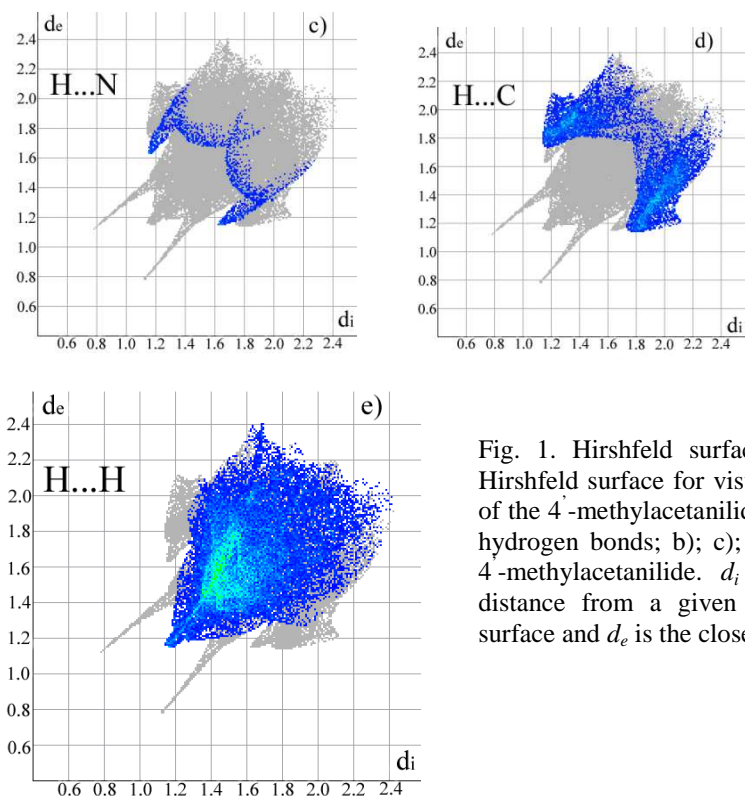
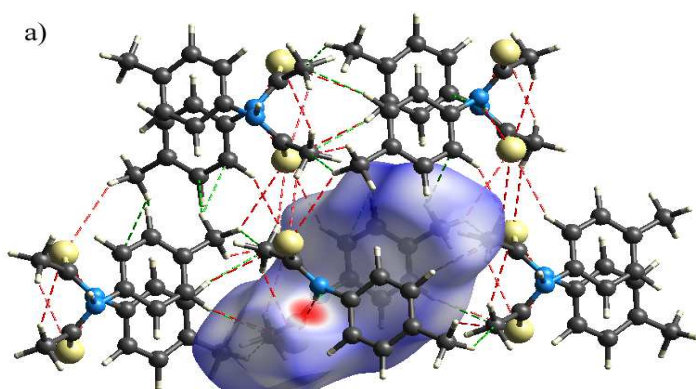


Fig. 1. Hirshfeld surface; a)  $d_{norm}$  mapped on Hirshfeld surface for visualizing the intercontacts of the 4'-methylacetanilide. Dotted lines represent hydrogen bonds; b); c); d); e) fingerprint of the 4'-methylacetanilide.  $d_i$  is the closest internal distance from a given point on the Hirshfeld surface and  $d_e$  is the closest external contacts.



Percentage of intermolecular contacts contributed to Hirshfeld surface

S ... H	21.0 %
N ... H	0.6 %
N ... C	1.0 %
H ... H	56.7 %
H ... C	19.5 %
C ... C	1.2 %

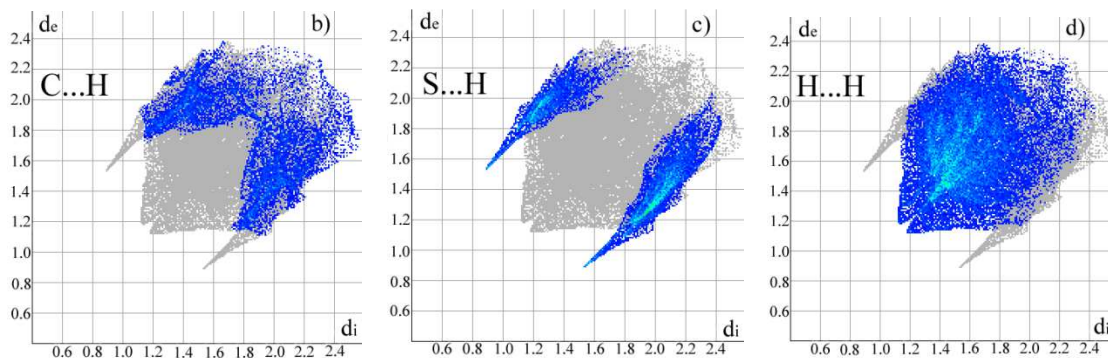


Fig. 2. Hirshfeld surface; a)  $d_{norm}$  mapped on Hirshfeld surface for visualizing the intercontacts of the 4'-methylthioacetanilide. Dotted lines represent hydrogen bonds; b); c); d) fingerprint of the 4'-methylthioacetanilide.

4'-methylthioacetanilide.  $d_i$  is the closest internal distance from a given point on the Hirshfeld surface and  $d_e$  is the closest external contacts.

### **Acknowledgement**

This work was funded by the grant of the Medical University of Silesia (No KNW-1-008/P/2/0).

All of the calculations were performed with the aid of hardware and software at the Wrocław Centre for Networking and Supercomputing WCSS, Wrocław, Poland.

# Hybrids of Cold Plasma Process with Graft Polymers and Nano Particles for Creating Functional Surface

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**Key words:** plasma, graft, functional surface, Nano Ag

Films deposited by cold plasma on the substrates have many advantages, such as good adhesion to substrate, excellent uniformity, easy preparation, thickness control, and pinhole free. The plasma polymerized films, as interface layers, can create wide application after post treatment. In this study, the surface of substrates was treated by cold plasma coating of hexamethyldisilazane(HMDSZ), Isopropanol or oxidation by O<sub>2</sub> to create various functional sites. We report some post treatment of various substrates, such as:

Part I: Surface-grafting polymerization of water soluble monomers.

1. Oxidation of surface (Titanium oxide films on polymer): the post plasma oxidation was attempted to reduce the organic residue of the TiO<sub>x</sub>-containing film on bamboo charcoal and enhance the ability of polarity gas adsorption,
2. Immobilization of Ionic Polymer / Nano-Silver Composite Hydrogels and Their Application.

Part II: Application of Atmosphere Plasma Treatment

1. Hydrophilic or hydrophobic surface modification
2. Surface-grafting polymerization of water soluble monomers

## **E-SCIENCE.PL: specialized web-based IT platform for polish scientific laboratories. Services for scanning microscopy, NMR, crystallography labs**

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**Keywords:** SPIN-LAB, E-SCIENCE.PL, LIMS, LABORATORIES

Project SPIN-LAB (Specialized Polish Scientific Infrastructure for Research Laboratories) is implemented by the Wrocław Centre for Networking and Supercomputing from April 2014 to end of November 2015. This project is based on knowledge, competence and experience in the field of efficient and safe processing, storage and sharing of data for the development of Polish science and innovation in the area of new research technologies. The main objective of the project is to modernize and improve the activities of Polish laboratories carrying out work within the framework of priority directions of scientific research of the country.

The project involves development of specialized, integrated IT platform for high -quality functions and features. Developed scientific platform E-SCIENCE.PL is a space dedicated to the scientific community for easy sharing, processing and secure data collection. It also enables easy and secure presentation and exchange of research results. The project is carried out by implementing a package of dedicated web-based services and applications for 20 leading Polish scientific institutions to support and improve the laboratory work. Main functionalities offered are as follows:

- Electronic Laboratory Notebook,
- Laboratory Management System,
- Implementation of *in-silico* experiments followed by data processing and visualization,
- Groupware tools for communication, bibliography and publications management,
- Information system of ongoing research projects and research results.

Among all scientific institutions chosen for this project are these who carry out crystallography, scanning microscopy, NMR research. The project offers individual solutions for laboratory. The main features for the application dedicated to crystallography, scanning microscopy, nmr research are secure and organized data collection, processing and management of experimental data and fast and easy data comparison for analysis and reports.

The result of the project will be the implementation of services and applications package accordant to the specific needs of individual scientific laboratories, which will allow for long-term use of modern research infrastructure, servers and High Performance Computing system without any additional costs. This will allow for more efficient and interdisciplinary cooperation among research centers, and at the same time strengthen the ability of individual research units.

**Acknowledgements:** Project co-financed by the European Regional Development Fund under the Innovative Economy Operational Programme (POIG.02.03.00-02-027/13).

Podziękowania: Projekt jest współfinansowany ze środków Europejskiego Funduszu Rozwoju Regionalnego w ramach Programu Operacyjnego Innowacyjna Gospodarka oraz z budżetu Państwa (nr POIG.02.03.00-02-027/13).

# Deep Eutectic Solvents, "Anionic Liquids"

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Deep Eutectic Solvents (DES) are a relatively new type of solvents typically made by mixing quaternary ammonium halides such as choline chloride with a hydrogen bond donor (HBD) such as urea, glycols, carboxylic acids etc. The anion plays a very important role as well as small amounts of added water. DES have already been used in a multitude of contexts such as vehicles for poorly soluble drugs, extractions, electroplating, biodiesel purifications, CO<sub>2</sub> absorption and many others.

The key feature of the freezing point depression is the interaction between the anion and the hydrogen bond donor. In the present case typically urea derivatives. This interaction is calculated as well as investigated by means of NMR. Deuterium isotope effects on chemical shifts is especially useful in this context<sup>1,2,3</sup>, but also one-bond NH couplings may be exploited.

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## Gas Phase NMR Experiments

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NMR spectroscopy in the gas phase delivers unique information on molecules free from intermolecular interactions when spectral parameters are extrapolated to the zero-density limit. Every such measurement is equivalent to the observation of an isolated molecule [1]. For example the gas phase results yield the precise values of spin-spin coupling and absolute shielding data that are useful in computational chemistry where they often permit us to judge the quality of numerous ab initio calculations. They also allow the experimental comparison of magnetic properties of two different nuclei at the stable external magnetic field when the two nuclei are in the same NMR sample. Assuming that the magnetic moment of a proton is well known and that the magnetic shielding of nuclei for small molecules can be precisely determined or calculated, it opens a way for the accurate determination of magnetic moments for many other nuclei [2]. The above method is limited by the number of gaseous compounds available for a comparison but due to high sensitivity of modern spectrometers it can be easily extended also to liquids when binary gaseous solutions are applied in the experimental studies [3]. The improved values of nuclear magnetic moments are essential for nuclear physics and different molecular spectroscopies. NMR experiment itself is based on the observation of nuclear magnetic moments and therefore the availability of nuclear magnetic moments may significantly change this method of spectroscopy. It is shown that the straightforward measurement of nuclear magnetic shielding is possible for many nuclei and can be used for the alternative standardization of NMR spectra [4]. It makes NMR spectroscopy more efficient, more universal and better connected with the quantum theory of shielding. This issue will be discussed in detail with some examples of general applications.

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# THEORETICAL STUDIES ON NMR PARAMETERS OF FREE AND CONFINED IN FULLERENES HD AND H<sub>2</sub> MOLECULES

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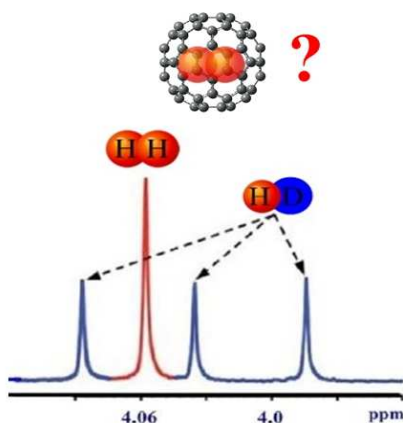
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**Keywords:** indirect nuclear spin–spin coupling constants; HD molecule; fullerene, DFT, CCSD(T)

## Abstract

In this work we reported on quantum-chemical prediction of nuclear magnetic shielding (and chemical shift) and indirect spin-spin coupling constant in free HD and H<sub>2</sub> molecules, as well as models of confined dihydrogen using the coupled cluster with single and double excitations (CCSD) and density functional theory (DFT) levels of theory. Inspired with the recent experimental NMR studies on HD and H<sub>2</sub> molecules confined inside C<sub>60</sub> fullerene we systematically investigated the sensitivity of <sup>1</sup>H nuclear magnetic shielding of H<sub>2</sub> and indirect spin-spin coupling constant <sup>1</sup>J<sub>HD</sub> in HD molecules to the interatomic separation in the gas phase, in the presence of benzene and inside fullerene cages of different size. The sensitivity of both NMR parameters to confinement is discussed in terms of very weak non-covalent interactions of HD and H<sub>2</sub> with fullerene cage.





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**Acknowledgements:** This work was supported by the GRAF-TECH/NCBR/10/29/2013 and partially by the Faculty of Chemistry, University of Opole (Grant 8/WCH/2015-S). M. J. is recipient of a Ph.D. scholarship under a project funded by the European Social Fund II". The calculation facilities and software in the Supercomputing and Networking Center ACK CYFRONET AGH in Krakow (PL-grid on zeus computer) and calculation facilities and software at the Supercomputing and Networking Center in Wrocław are also acknowledged.

# EFFICIENT MODELLING OF STRUCTURAL AND SPECTROSCOPICAL PARAMETERS OF NANOCARBONS

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For over twenty years fullerenes, carbon nanotubes (CNTs), and recently graphene, have been considered promising materials in electronics and material sciences. Pristine CNTs, as well as other functionalized tubes, are used in several fields of research and industry. Due to their tubular morphology, CNTs can serve as reactors for nanoscale chemical reactions. Open-ended CNTs have been a subject of many studies as model systems, for example encapsulated simple molecules inside the nanotube has served for interaction, density or proton transfer studies. Recently, the efficacy of targeted medical therapies has improved through the use of nanoparticles that can package drugs with a controlled shape, size, and surface chemistry to enhance their solubility, bioavailability, and/or residence times. An ancillary benefit of using nanoparticles is that many can additionally serve as a stable imaging label (Raman agent). Due to growing demand for well-characterized nanomaterials and often insufficient use of spectroscopic techniques (e.g. NMR) for their characterization we proposed efficient theoretical modeling of structural, energetic and spectral properties ( $^{13}\text{C}$  NMR chemical shifts, Raman bands) of several real-size CNTs to enhance experimental spectra interpretations.

We also concentrated on theoretical modeling of endohedral fullerenes that have an atom, ion, molecule or a cluster enclosed inside the cage. The field of endohedral metallofullerenes (EMF), where a metal or metal-based clusters are encapsulated, has undergone through rapid development, because of their interesting molecular properties, unusual bonding patterns, and potential practical applications, especially if actinides are encased. So far, the only more experimentally (UV/vis/NIR, XANES) characterized actinide EMFs are  $\text{U@C}_{82}$  and  $\text{Th@C}_{84}$ , studied by Akiyama et al.<sup>1</sup> However, the results for  $\text{Th@C}_{84}$  are difficult to interpret. The typical oxidation state Th is +IV but that could not be fully confirmed by the XANES spectra, because the corresponding absorption edge was found less reductive than in  $\text{Th}^{\text{IV}}(\text{NO}_3)_4$  suggesting a possibility of  $\text{Th}^{\text{III}}$  but any materials with  $\text{Th}^{\text{III}}$  providing a comparison could not be found. Based on this it was concluded that the  $\text{Th@C}_{84}$  is probably a  $\text{Th}^{\text{IV}}@C_{84}$  system. Notably, this possibility does not have any experimental precedence in the literature. Up to date experimentally reported mono-metal  $\text{M@C}_{84}$  compounds found in the literature contain divalent metal, such as isomers of  $\text{Sm@C}_{84}$ . No experimentally confirmed trivalent or tetravalent analogues could be found in the literature. Hence,  $\text{Th@C}_{84}$  presents very probably a new type of the  $\text{M@C}_{84}$  system, worth of further investigations.

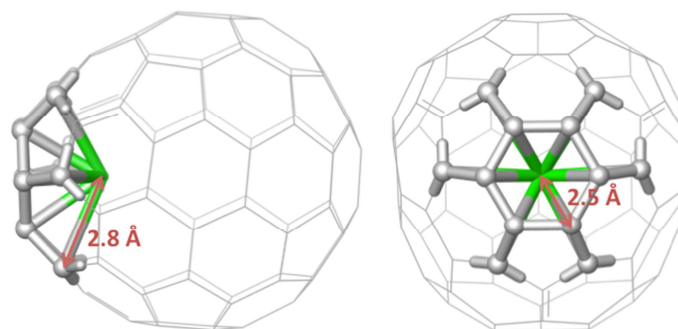


Figure. The PBE0/def2-TZVPP optimized Th@C<sub>84</sub> structure of isomer No.10. Two different C-Th “quasi-bond” distances are depicted.

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The work was supported by the Czech Science Foundation (Grant No. 14-03564S).

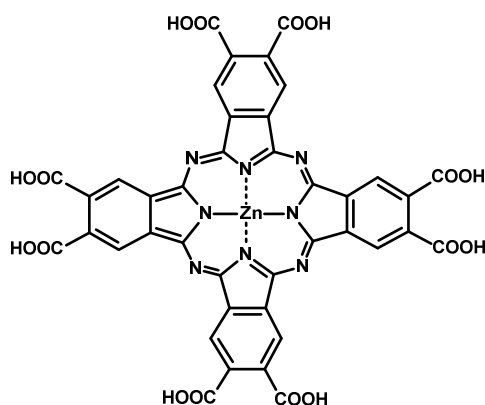
# Interactions of zinc octacarboxyphthalocyanine with selected amino acids - theoretical calculations

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**Keywords:** Phthalocyanines, Zinc octacarboxyphthalocyanine, Amino acid, UV-Vis spectra, Theoretical calculations

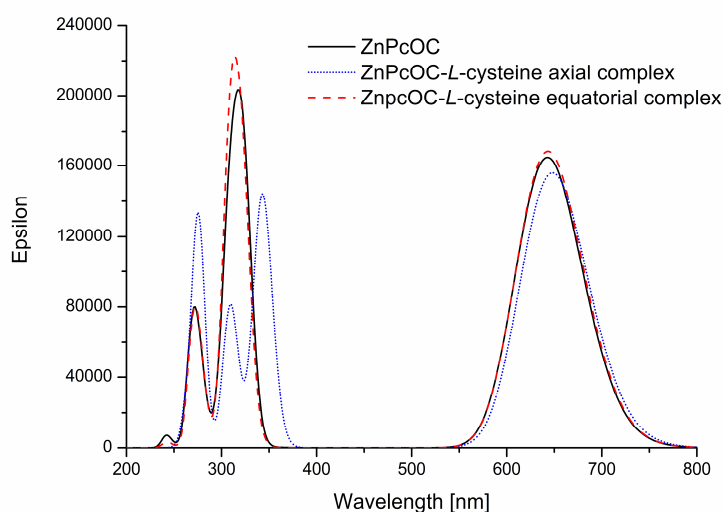
Phthalocyanines (Pcs), which are considered to be synthetic porphyrin analogs, belong to an important group – aromatic macrocycles that have a conjugated system containing 18 delocalized  $\pi$  electrons [1–3]. Due to the presence of four isoindole nitrogen atoms phthalocyanine ligand can create a chelate bonds with different metals [1]. Phthalocyanines found many practical applications due to their specific physicochemical properties [4]. 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 [5]. Recently, much attention has been paid to the possibility of using these compounds as second generation photosensitizers in photodynamic therapy (PDT) [6,7]. 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 neoplastic cells [5, 8, 9]. The subject of our research is zinc phthalocyanine (ZnPcOC) that have eight carboxylic groups attached to the benzene rings (Fig. 1) what make the compound well soluble in water. The study of water-soluble phthalocyanines is of great theoretical and practical significance.



**Fig. 1.** Structure of zinc octacarboxyphthalocyanine, ZnPcOC.

All calculations were performed using the Gaussian 09 program [10]. Theoretical calculations methods were used to investigate the problem of the interactions of zinc octacarboxyphthalocyanine (ZnPcOC) with the selected amino acids

(glycine, *L*-histidine, *L*-cysteine, *L*-serine, *L*-tryptophan). The geometric structures of the axial and equatorial complexes ZnPcOC: amino acids were optimized by B3LYP/6-31G(d) method and analyzed in terms of the properties of stabilizing them interactions. The energy of interaction was evaluated from energy differences between complex and its individual components and was corrected using the counterpoise (CP) method. Using time dependent density functional theory (TD-DFT) method we showed the impact of two types of complex formation on the electronic absorption spectra (Fig. 2). UV/Vis spectra were calculated from fully optimized geometry at B3LYP/6-31G(d) level of theory.



**Fig. 2.** TD-DFT/CAM-B3LYP/6-31G(d) calculated UV–visible spectra of zinc octacarboxyphthalocyanine and its axial and equatorial complexes with *L*-cysteine.

**Acknowledgements:** Marta Kliber-Jasik is a recipient of a Ph.D. scholarship under a project funded by the European Social Fund. Calculations were carried out in the Academic Computer Centre CYFRONET, AGH, Kraków.

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# Fragmentation Techniques – a Step Towards Linear Scaling in Computational Chemistry

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**Keywords:** linear scaling methods, elongation method, cutoff technique, fragmentation methods, charge sensitivity analysis

Huge progress in computer technology brings about conditions for *ab initio* computational methods to be of practical value in chemistry, biochemistry and material science. However, the application of Hartree-Fock (HF), Kohn-Sham (KS), and post-HF computational methods to huge molecular systems is limited due to undesired scaling behavior. The expense of a given method is usually expressed as  $\beta N^\alpha$ , where  $N$ ,  $\alpha$ , and  $\beta$  are the number of basis functions applied in the calculations, scaling exponent, and scaling prefactor, respectively. In this presentation we would like to describe the elongation (ELG)<sup>1</sup> and elongation/cutoff (ELG/C) methods and their scaling behavior.

The ELG and ELG/C methods belong to fragmentation techniques. They are based on concept of locality and take into account the sparsity of HF and KS matrices in regionally localized molecular orbital basis set. In this presentation, a recent progress in ELG (ELG/C) method is summarized. Namely, a simple way of including long-range polarization into ELG (ELG/C) methods is presented. The modified ELG method includes a simplified electrostatic field resulting from point-charge distribution of the system's environment. The field attenuates during the ELG process to eventually disappear when the final structure is reached. The point-charge distributions for each ELG step are obtained from Charge Sensitivity Analysis (CSA) in force-field atoms resolution. The presence of the intermediate field improves the accuracy of ELG calculations. The errors in total energy and its kinetic and potential contributions are reduced by at least one-order of magnitude.

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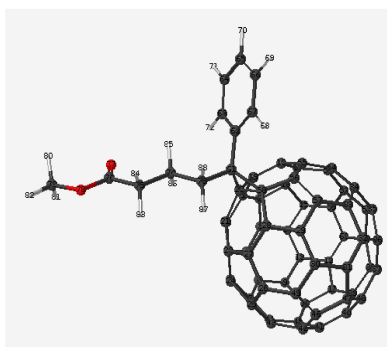
# INTERMOLECULAR INTERACTIONS AND ELECTRON EXCITATIONS IN COMPLEXES WITH PCBM

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**Keywords:** SAPT(DFT), TD-DFT, charge-transfer, PCBM, solar cell

The [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) molecule is a popular acceptor in photocurrent generating junctions, where it coexists in a complex with a donor molecule. It is therefore of interest to examine the strength and physical nature of intermolecular interactions in complexes containing PCBM, as well as to investigate lowest electronically excited states of such complexes, paying special attention to charge-transfer states with nonzero oscillator strength, which can play a role in the photocurrent generation. In this contribution SAPT(DFT) and TD-DFT methods were used for these studies. The PCBM molecule is examined either in complexes with small molecules, like benzene or porphyrin [1], or with a newly synthesized 25Th-cardo polyazomethine (PAZ) [2]. In the latter case a detailed comparison with the experimental data is reported, too.



**Fig. 1** The PCBM molecule

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# NMR ANALYSIS OF ECONAZOLE - COMPUTATIONAL CALCULATIONS IN CHEMICAL ENVIRONMENT

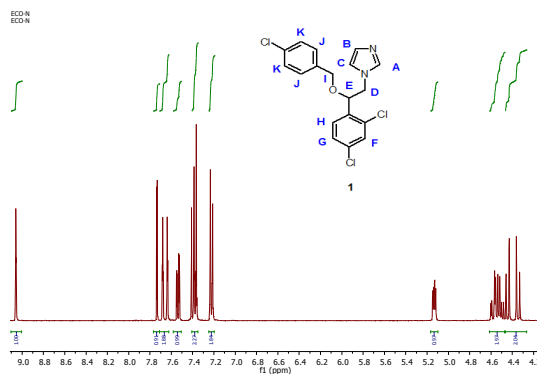
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**Keywords:** econazole, NMR calculations, chemical shifts, DFT, GIAO, QTAIM

Imidazole derivatives are used mainly as antifungal, antibacterial and antiprotozoal agents. As antifungal drugs, imidazole derivatives inhibit the synthesis of normal membrane sterols in fungi [1]. One of the most important compounds among antifungal imidazoles is *econazole* nitrate **1** (**Fig. 1**). Continuing our investigations on the interactions of biologically important azahetarenes with the environment [2,3], we focused our attention on the <sup>1</sup>H NMR spectral analysis of **1**. The calculated chemical shifts (GIAO method; *Gaussian G09 D.01* software) were correlated with experimental data (**Fig. 1**) using the DFT formalism and B3LYP/6-31G(d,p), CAM-B3LYP/6-31G(d,p), B3LYP/6-311+G(d,p) and PBE1PBE/6-31G(d,p) approaches both in gaseous phase, as well as the CPCM solvation model and water as solvent. The B3LYP/6-311+G(d,p)/CPCM approach (**Tab. 1**), as well as the PBE0/CPCM functional revealed a stronger correlation of the NMR spectrum with the corresponding experimental one, i.e. lower values of the relative percentage errors and mean absolute deviation parameters (MAD=0.40 and 0.41 respectively). The application of the CPCM solvation model **1** resulted in an improvement of the relative percentage errors of the chemical shifts of the protons A-K when compared to the rotamers optimized in the gaseous phase. The higher values of the relative percentage errors of the protons A and D however were caused by significant short C<sub>arom</sub>-H...H<sub>2</sub>C contact and undergoing shielding due to the steric hindrance between interacting moieties. This assumption was also proved by MEP, NBO, and the QTAIM calculations (*AIMAll version 14.11.23* software).



**Fig. 1.** The experimental <sup>1</sup>H NMR of the econazole (**1**).

**Tab. 1.** Calculated and experimental data for **1**; the following parameters were determined for their proton groups: experimental (Exp.) and calculated values of the chemical shifts of rotamers (I-V), partial absolute errors ( $\delta 1$ - $\delta 5$ ) and average absolute error ( $\delta$ ), relative percentage errors (E); calculated NMR shielding for proton  $H_{ref} = 31.9753$  ppm for TMS (B3LYP/6-311+G(d,p)/GIAO/CPCM; MAD = 0.40.

Protons	Exp.	I	II	III	IV	V	$\delta 1$	$\delta 2$	$\delta 3$	$\delta 4$	$\delta 5$	$\delta$	E
<b>A</b>	9.059	7.833	7.530	7.532	7.631	7.836	1.226	1.529	1.526	1.428	1.223	1.386	<b>15</b>
<b>B</b>	7.680	7.190	7.331	7.331	7.321	7.195	0.491	0.349	0.350	0.359	0.485	0.407	<b>5</b>
<b>C</b>	7.637	7.227	7.558	7.558	7.262	7.244	0.410	0.080	0.080	0.376	0.394	0.268	<b>4</b>
<b>D</b>	4.554	3.989	3.955	3.954	3.871	3.982	0.565	0.599	0.600	0.683	0.572	0.604	<b>13</b>
<b>E</b>	5.133	5.124	4.898	5.259	4.967	5.088	0.010	0.235	0.126	0.166	0.045	0.116	<b>2</b>
<b>F</b>	7.735	7.690	7.658	7.784	7.592	7.696	0.045	0.077	0.049	0.143	0.039	0.071	<b>1</b>
<b>G</b>	7.396	7.746	7.482	7.679	7.541	7.744	0.350	0.087	0.284	0.146	0.349	0.243	<b>3</b>
<b>H</b>	7.537	8.080	7.992	8.216	7.893	8.084	0.543	0.455	0.679	0.356	0.547	0.516	<b>7</b>
<b>I</b>	4.395	4.176	4.116	4.219	4.209	4.173	0.219	0.279	0.176	0.186	0.223	0.216	<b>5</b>
<b>J</b>	7.376	7.664	7.350	7.542	7.485	7.673	0.288	0.026	0.166	0.109	0.297	0.177	<b>2</b>
<b>K</b>	7.225	7.696	7.549	7.626	7.506	7.700	0.471	0.323	0.401	0.280	0.474	0.390	<b>5</b>

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## Water in Porous systems. Toward controlling water imbibition to model white hardened cement paste and diffusion of water and salt (NaCl) into concrete

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In this paper we will discuss basic ideas of interactions between water and porous systems. These processes are related to low resistance of concrete to water and corrosive action of salt.

We will show the results of experimental NMR studies (<sup>1</sup>H, <sup>2</sup>H, <sup>21</sup>Na NMR) related to water penetrating large, medium and small pores in model hardened white cement paste.

Among several ways of controlling water penetration by applying specific additives in powdered form or mixed with water during concrete production we will concentrate on “**Hydrozol K**” – a formulation designed same time ago in Opole (High Engineering School). We will also discuss on a “**Dezodor**” formulation that is helpful in controlling bacteria and pests in environmental problems.



Fig. 1. Two models of porous systems: (left) Swiss cheese and (right) a sponge

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# SBA-15 mesoporous silica free-standing thin films activated by copper ions - preparation and characterization

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## *Abstract*

The present work is devoted to SBA-15 silica thin films containing copper ions anchored inside channels via propyl phosphonate groups. The materials has been prepared in the form of thin films with hexagonally arranged pores, laying rectilinear to substrate surface. The films, that are presented in the present work, has been prepared in the free-standing form. The structural properties of the samples has been investigated by X-ray re- fractometry, atomic force microscopy (AFM) and transmission electron microscopy (TEM). The molecular structure has been investigated by Raman spectroscopy supported by DFT numerical simulations. On the base of varied out researches we was able to determinate of the pores arrangement and verify of activation process related to phosphonate groups in unambiguous way.

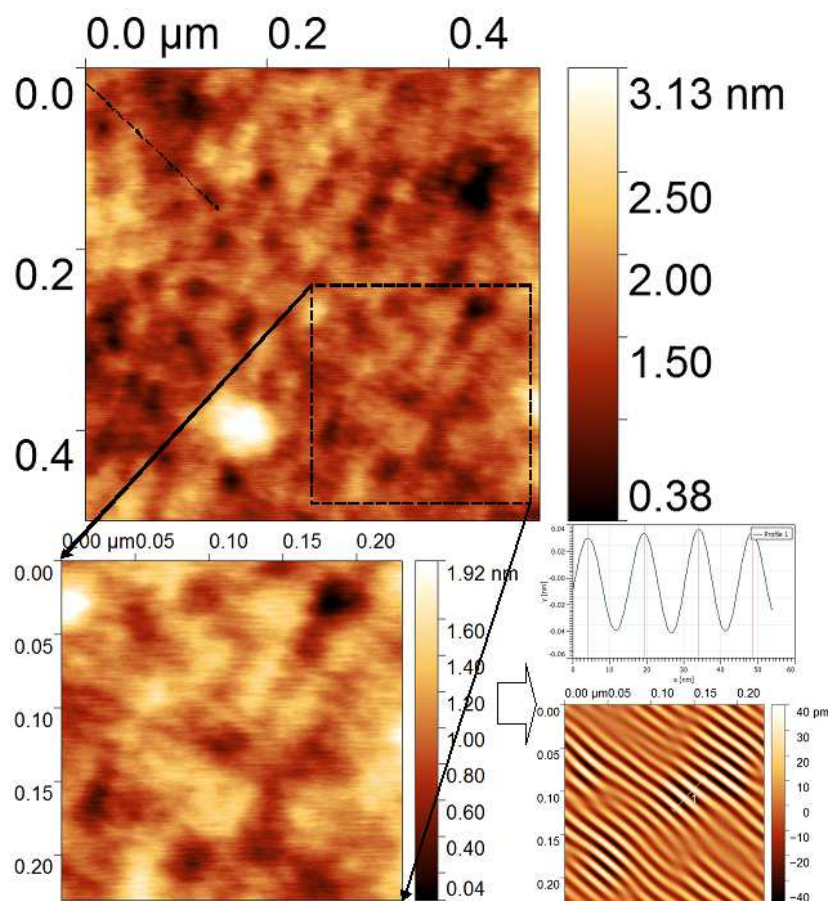


Fig. 1. The AFM microphotographies of the SBA-15 thin film activated by copper ions.

# Electrochemical Supercapacitor Behaviors Of Nano Iron Oxide/Polyaniline/Reduced Graphene Oxide Hybrid Materials

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**Key words:** supercapacitor, reduced graphene oxide, iron oxide, polyaniline

Integrated supercapacitors with extended operation voltage are important for high energy density storage devices. Supercapacitors store energy using either ion adsorption (electrochemical double layer capacitors) or fast surface redox reactions (pseudo-capacitors). They can complement or replace batteries in electrical energy storage and harvesting applications, when high power delivery or uptake is needed.

If we integrate the electrochemical double layer and pseudo capacitors, it will enhance the properties of supercapacitors. In this study, the polyaniline, iron oxide and reduced graphene oxide are hybrid to enhance the performance of supercapacitors and form new innovated supercapacitors. These new hybrid materials are examined by XRD, SEM, TEM, TGA, FTIR, ICP and electrochemical analysis. The results of electrochemical test show that 50wt%PANI/RGO has the best electrochemical performance and has the specific capacitance of 268 F/g in 10 cycles test. The specific capacitance of 50wt%PANI/RGO is better than that of RGO (165 F/g) or PANI (131 F/g). In Fe<sub>3</sub>O<sub>4</sub>/RGO system, 10wt%Fe<sub>3</sub>O<sub>4</sub>/RGO has best specific capacitance 240 F/g in 10 cycles test. The result is better than that RGO (165 F/g) or Fe<sub>3</sub>O<sub>4</sub> (4.4 F/g). The results of this study indicated new hybrid material system has potential to apply in the integrated supercapacitor devices. For the 10wt%Fe<sub>3</sub>O<sub>4</sub>/45wt%PANI/RGO sample, the specific capacitor of 341 F/g can be obtained in 10 cycles. Its electrochemical performance is better than that of PANI/RGO or Fe<sub>3</sub>O<sub>4</sub>/RGO systems. This study indicates the innovated hybrid Fe<sub>3</sub>O<sub>4</sub>/PANI/RGO material system have the potential to apply in supercapacitor in near future.

# HYDROGEN BONDS IN COMPLEXES OF SECONDARY AMINES WITH DIMETHYL SULFOXIDE AS STUDIED BY SOLUTION NMR, DFT AND AIM CALCULATIONS

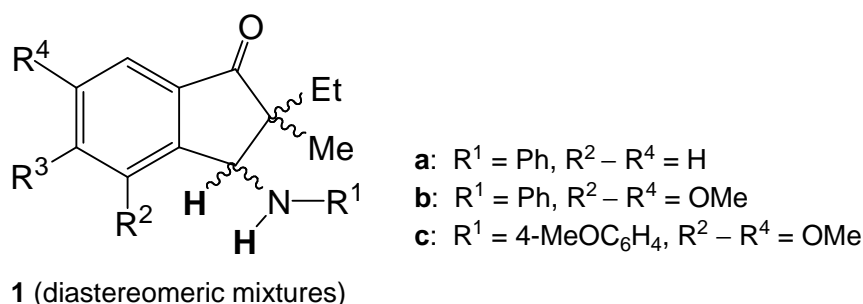
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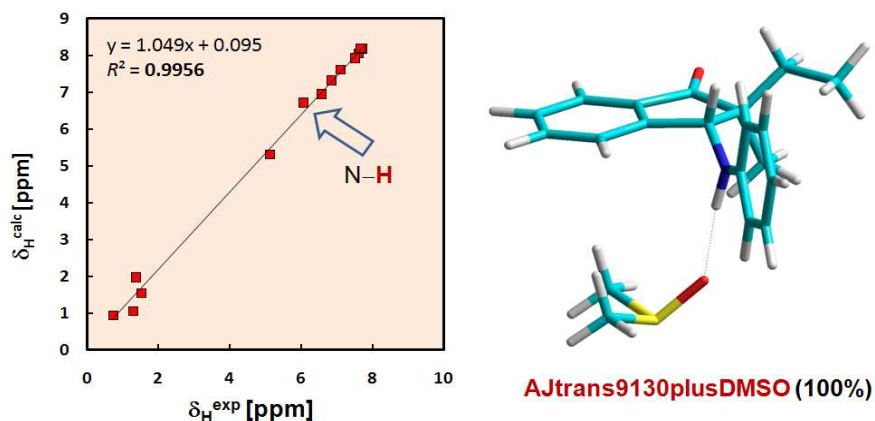
**Keywords:** Hydrogen bonds; Complexes; Secondary amines; DMSO; Solution NMR; DTF; NMR calculations; AIM analysis

Dimethyl sulfoxide is the NMR solvent of choice for many organic compounds due to its excellent solubility properties for protic and charged molecules, which are insoluble in CDCl<sub>3</sub>. Although the effects of modification of <sup>1</sup>H NMR spectra of hydroxy compounds in DMSO-*d*<sub>6</sub> are well recognized [1], the nature of related complexes formed in solution is not finally established. Similar interactions with amines are still less known. In our works on *N*-substituted isoindolinones a few amino derivatives **1a-c** (see Fig. 1) were synthesized [2, 3], forming 1:1 complexes of type >N-H···O=S(CD<sub>3</sub>)<sub>2</sub> as was evidently manifested by relative large <sup>3</sup>J<sub>H-C-N-H</sub> couplings (*ca.* 10 Hz) observed in their <sup>1</sup>H NMR spectra recorded in DMSO-*d*<sub>6</sub>.

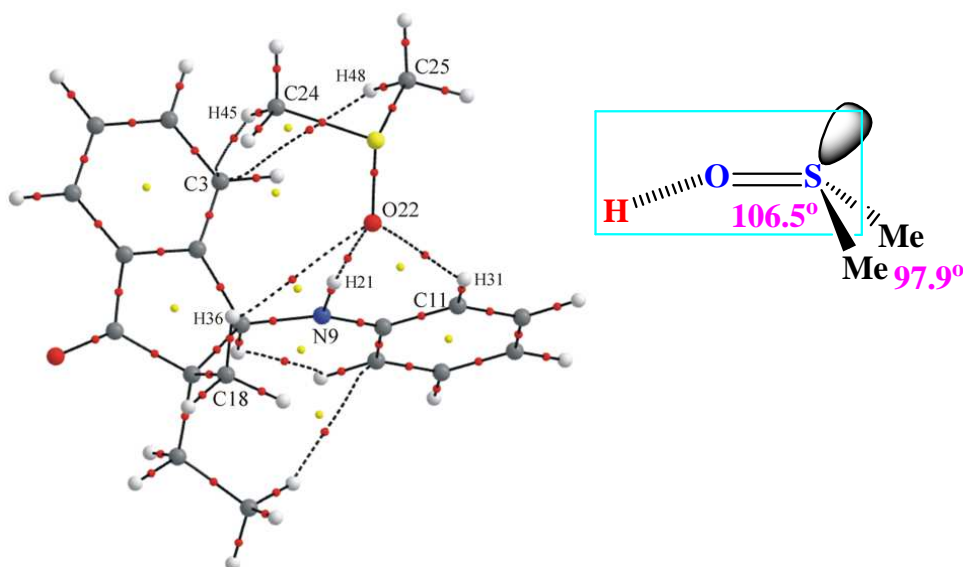


**Fig. 1.** The family of compounds under study.

An intermolecular H-bonding in these complexes was analyzed in detail for a mixture of two diastereomeric secondary amines **1a** isolated with a *trans/cis* ratio of ~1.4:1. The results of our investigations [modeling of the structures at the B3LYP/6-31+G(*d,p*)/IEF-PCM(DMSO) level followed by adequate single-point calculations of NMR parameters ( $\delta_{\text{H}}$ ,  $\delta_{\text{C}}$  and  $J_{\text{HH}}$ ) and topological ‘Atoms in Molecules’ analysis (see Fig. 2) of existing H-bond networks] will be presented in detail on the poster.



**Fig. 2.** Reproduction of the experimental  $\delta_{\text{H}}$  data by using only one complex **1a**–DMSO (form AJtrans9130&DMSO) (*left*) and its drawing (*right*).



**Fig. 3.** A molecular graph of the complex **1a**–DMSO (form AJtrans9130&DMSO) according to an AIMAll [4] depiction (*left*) and a schematic representation of the geometry of the constituent H-bonded molecule of DMSO (*right*).

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# PLGrid Infrastructure. Solutions For Computational Chemistry

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**Keywords:** computational chemistry, grid infrastructure, efficient computations

PLGrid infrastructure and PLGrid Core[1] and PLGrid NG[2] projects are aimed to provide Polish researches with powerful computational infrastructure which is also tailored to the needs of specific scientific communities. Moreover, it also addresses 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 computational chemists are organized within the Quantum Chemistry and Molecular Physics domain. Among services provided for computational chemistry is InSilicoLab for Chemistry[3] web portal which eases usage of grid infrastructure for chemical calculations.

All services and solutions available in PLGrid infrastructure are constantly developed and have got robust and continuously updated technical documentation[4,5]. Users could obtain detailed information and help about efficient execution of their scientific problems from our domain specific experts through web based Helpdesk[5]. Moreover, all computing centres involved in PLGrid infrastructure provide vast portfolio of free trainings for scientific users.

## References

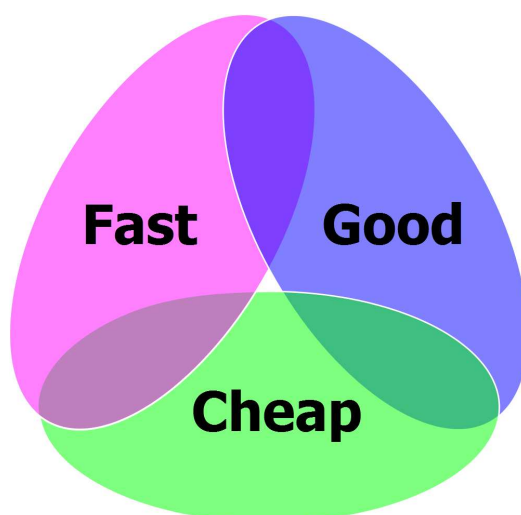
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# “BENDING THE IRON TRIANGLE (WITH MOORE’S LAW HELP)” – SIMPLIFICATIONS AND COMPROMISES IN COMPUTATIONAL CHEMISTRY

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**Keywords:** computational chemistry, DFT, molecular dynamics, semiempirical methods.

Computational Chemistry is just about as old as computers are. Both are evolving at a fast pace, however the road to improvement takes unexpected turns. Is the ever-enlarging applicability area of computational methods just caused by Moore’s law? The key to success seems to lie not only in increase of computing power available, but also in algorithm optimization and simplification related issues. Linear scaling quantum semiempirical methods and reactive force fields serve as examples.



# MOLECULAR ELECTRIC PROPERTIES OF SUBSTITUTED CARBAZOLE

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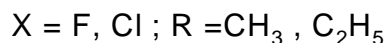
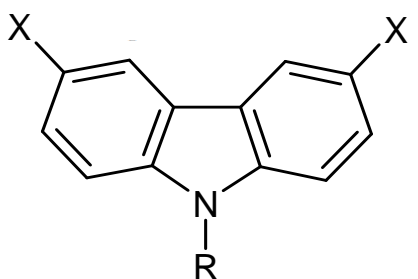
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**Keywords:** carbazole, hyperpolarizability, nonlinear optics (NLO), DFT, CCSD

Electric properties of molecules, especially higher-order response properties like hyperpolarizabilities ( $\beta$  and  $\gamma$  tensors) are of particular interest in designing materials with large nonlinear optical (NLO) properties [1]. Frequency-dependent response properties allow more realistic description of NLO experiments and are of fundamental importance in understanding molecular spectra.

In this work we report on the prediction of static and dynamic electric properties of carbazole and its halogenated derivatives (Figure 1). The static electric properties have been calculated with the B3LYP and CAM-B3LYP functionals using Pol and Z3Pol basis sets [3,4] and compared to the CCSD results. Dalton 2013 [5] for CCSD data, and Gaussian09 [6] suite of programs for dynamic results have been used in this work.



**Fig. 1.** General scheme of carbazole and its 3,6 – dihalogenated derivatives.

DFT values of dipole moments and static polarizability components agree very well with the CCSD results (Table 1), while disagree for hyperpolarizabilities, especially for the second hyperpolarizability ( $\gamma$ ). For  $\gamma$  hyperpolarizability B3LYP and CAMB3LYP are only in fair agreement with each other. CAMB3LYP/Z3Pol combination seems to be a promising tool for providing reliable static and dynamic electric response properties up to the first hyperpolarizability ( $\beta$ ) tensor.

**Tab. 1.** Dipole moment, polarizability and hyperpolarizabilities of carbazole. Z3Pol basis set, geometry optimized at the B3LYP/aug-cc-pVTZ level. All entries in a.u.

Property	B3LYP	CAM-B3LYP	CCSD
$\mu_z$	0.6351	0.6194	0.6157
$\alpha_{xx}$	77.84	77.18	81.54
$\alpha_{yy}$	235.5	226.9	228.5
$\alpha_{zz}$	152.3	150.1	153.1
$\alpha_{av}$	155.2	151.4	154.4
$\beta_{zzz}$	29.6	30.7	55.9
$\beta_{zxx}$	32.5	29.5	35.4
$\beta_{zyy}$	183.2	176.5	252.7
$\beta_{ll}$	187	142.0	206.4
$\gamma_{xxxx}$	23510	17430	19730
$\gamma_{yyyy}$	151070	113890	149270
$\gamma_{zzz}$	28650	22810	28550
$\gamma_{ll}$	59230	44860	57340

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# **Endohedral hydrogen fullerenes: where theoretical calculations are in line with experimental results**

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## **Abstract**

Soon after Kroto and his group postulated the possibility of encapsulation of La atoms inside C<sub>60</sub> cage [1], numerous experimental and theoretical studies have been carried out in order to understand the forms and characteristics of endohedral complexes [2]. Of particular importance, endohedral hydrogen fullerenes have received much attention with regard to their possible usage as hydrogen carriers [3]. However, determination of the exact number of hydrogen molecules that can be encapsulated inside fullerenes' cages remains controversial [4,5].

Working on selected fullerene cages, we have carried out systematic calculations at various theoretical levels, in order to determine the encapsulation limit, and to clarify the reasons based on which the “exaggerated” number of hydrogen molecules have been reported [6,7].

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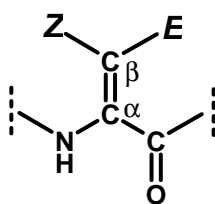
# $\alpha,\beta$ -DEHYDROAMINO ACIDS IN NATURALLY OCCURRING PEPTIDES

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**Keywords:** dehydroamino acids, peptides, bioactivity

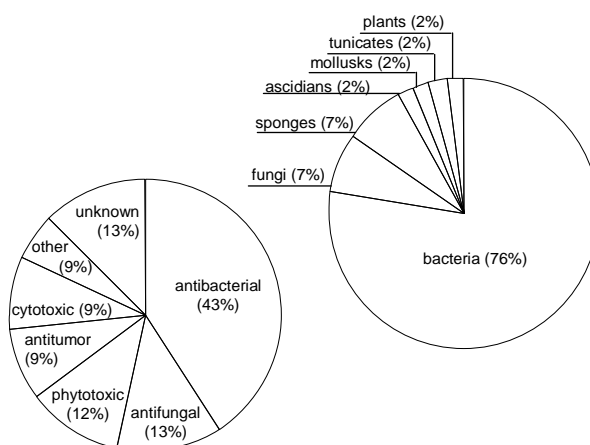
$\alpha,\beta$ -Dehydroamino acids are naturally occurring non-coded amino acids, found primarily in peptides (Figure 1).



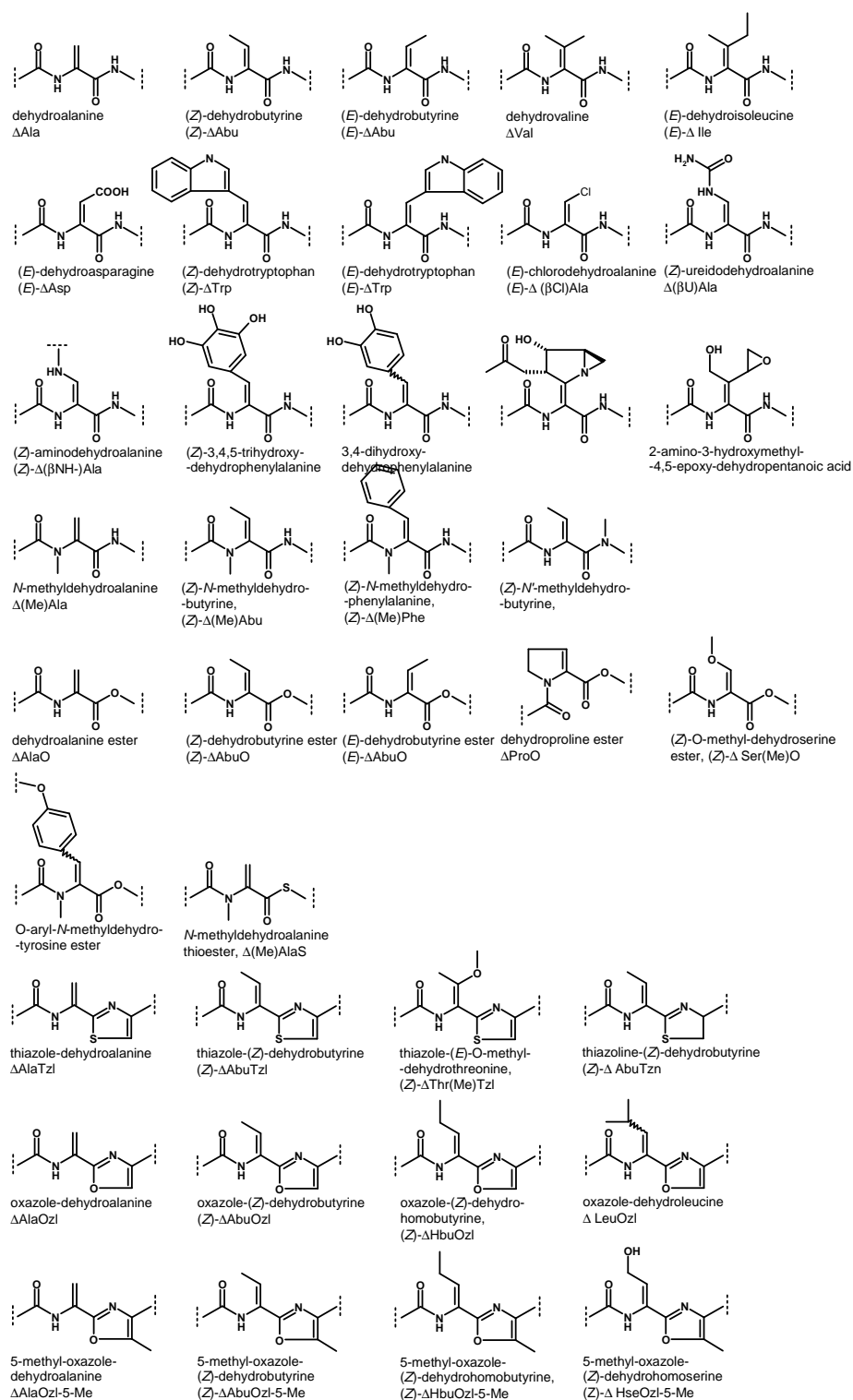
**Fig. 1.** General scheme of  $\alpha,\beta$ -dehydroamino acid residue.

Dehydropeptides are isolated primarily from bacteria, less often fungi, marine invertebrates or even higher plants. They reveal mainly antibiotic, antifungal, antitumor, and phytotoxic activity (Figure 2). The collected data shows the relation between the structure and bioactivity. It also enables to estimate the activity of compounds, which were not studied in this field, but which belong to a larger peptide family to be predicated. A few examples show that the type of the geometrical isomer of the  $\alpha,\beta$ -dehydroamino acid residue can be important or even crucial for biological activity.

The presented review shows 42 different naturally occurring  $\alpha,\beta$ -dehydroamino acid residues. The structural differences cover various side chains, including *Z* and *E* isomers, as well as three and main chain modifications: methylation of peptide bond, introduction of ester group and heterocyclic ring (Figure 3). More than 60 different structures of dehydropeptides were classified, which often cover broad families of peptides.



**Fig. 2.** Source of origin and bioactivity of peptides containing the  $\alpha,\beta$ -dehydroamino acids.



**Fig. 3.** Various structural units of the  $\alpha,\beta$ -dehydroamino acids found in natural peptides. This includes, variations of the side chains, geometrical isomers, modification of main chain, and their combination.

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## MOLECULAR MODELING OF SWCNTs $^{13}\text{C}$ NMR CHEMICAL SHIFTS

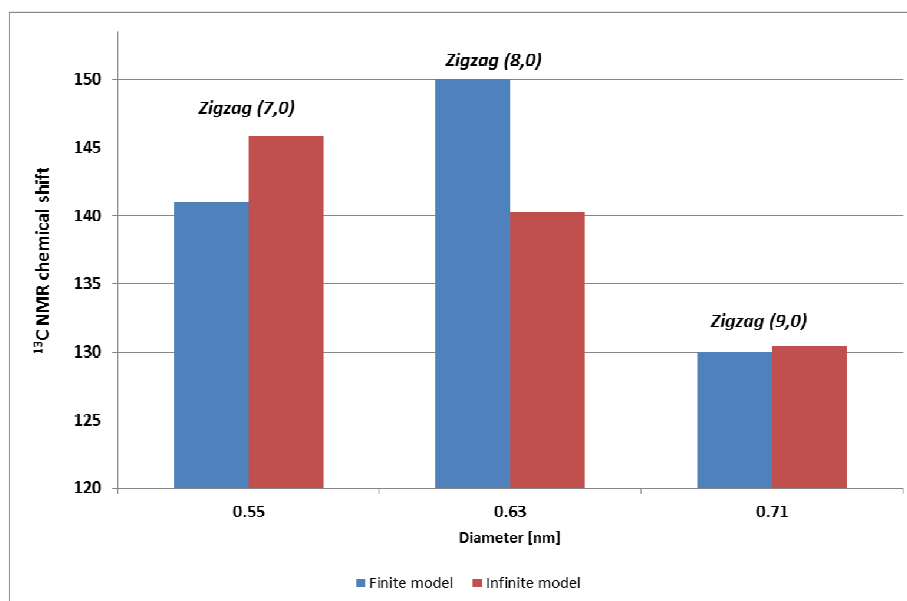
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**Keywords:** SWCNT;  $^{13}\text{C}$  NMR; chemical shift; DFT; carbon nanotubes

### Abstract

In this work we have compared theoretical  $^{13}\text{C}$  NMR chemical shifts (in ppm) for selected finite and infinite simplified models of single wall carbon nanotubes (SWCNTs). For finite models we used density functional theory and recently designed #STO-3Gmag basis set (from Leszynski group) and for infinite models the PBE density functional and plane wave basis sets. The obtained results were compared with available experimental results for the similar diameter SWCNTs.



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# CONFORMATIONAL PROPERTIES OF OXAZOLE-AMINO ACIDS AND THEIR ANALOGUES

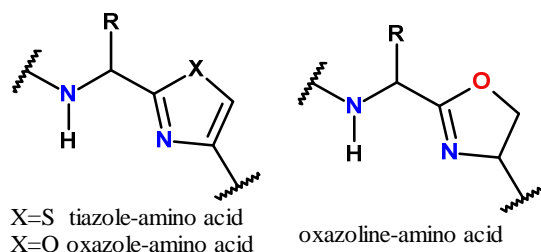
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**Keywords:** DFT, conformation, Ramachandran diagram, non-standard amino acid, hydrogen bond

Properties of proteins and peptides depend on their spatial arrangement - conformation. The presence of non-standard amino acid residues in the peptides causes that they have new and unusual properties. In last decade many macrocyclic peptides (tiopeptide antibiotics or alkaloids) were found, which consist of amino acids residues with a heterocyclic ring in place of the C-terminal amide. Some of these residues have additionally a double bond between the carbon atoms  $\alpha$  and  $\beta$ , too. Such amino acids are called  $\alpha,\beta$ -dehydroamino acids. These peptides, produced mainly by bacteria and sponge, reveal antibacterial, antitumor or antiparasite activities.

A series of non-standard amino acids with oxazole (Ozl), thiazole (Tzl) and oxazoline (Ozn) (Fig. 1) were investigated using theoretical (DFT, mainly M06-2X) and experimental methods (NMR-NOE, IR, X-ray crystallography), including a review of Cambridge Structural Database. The conformational tendency of the model compounds in solution and solid state were defined.



**Figure 1** Non-standard amino acids with heterocyclic ring

Presence of heterocyclic ring changes conformational properties of the studied amino acids in comparison to the standard amino acids. Heterocyclic ring causes that the amino acids have tendency to adopt the conformation  $\beta_2$  ( $\phi, \psi \sim 180^\circ, 0^\circ$ ) - unusual for the standard amino acids. The conformation  $\beta_2$  is stabilized by N-H $\cdots$ N hydrogen bond formed between N-terminal amide group and the nitrogen atom of the heterocyclic ring, which is much stronger than the N-H $\cdots$ O hydrogen bond in the conformation C5. The power of these hydrogen bond in these residues can be explained by the electron density distribution around the hetero atoms in the heterocyclic ring, which differs from the amide group. For dehydroamino acids this tendency is much stronger, because of presence of  $\pi$ -electron conjugation and shorter N-H $\cdots$ N hydrogen bond, and it does not depend on type of the side chain.

The tendency to adopt the conformation  $\beta_2$  decreases with increasing polarity of environment for all investigated compounds. In more polar environment the conformations  $\beta$  (for the amino acids with oxazole and thiazole) or  $\alpha_R$  (for oxazoline-amino acids) are preferred.

Thiazole, oxazole, and oxazoline-amino acids have rather similar conformational profile, although some differences were found. Oxazole and thiazole ring have little aromatic character in which both the nitrogen and hetero atom are involved. The hetero atom shares its electron pair with aromatic sextet, as a consequence, it should be weaker hydrogen bond acceptor than nitrogen, which has lone electron pair. As a result the aromatic character, the oxazole and thiazole rings are plane in contrast to oxazoline ring. In oxazoline ring occurs two carbon atoms with the  $sp^3$  hybridization and the peptide which includes this ring never will be plane.

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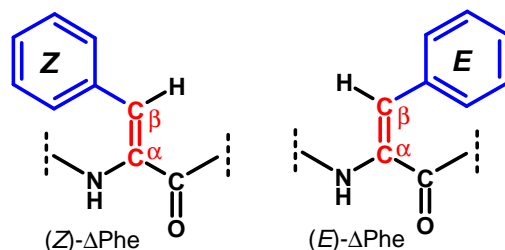
# CONFORMATIONS DIFFERENCES BETWEEN ISOMERS *Z* AND *E* OF DEHYDROPHENYLALANINE

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**Keywords:** dehydroamino acids, dehydrophenylalanine, conformations, hydrogen bond

Geometrical isomerism *Z/E* constantly attracts attention because the same chemical composition but different position of atom in space generates different chemical properties [1]. In natural peptides the isomerism *Z/E* is represented by  $\alpha,\beta$ -dehydroamino acids, and there are examples which shows profound effect of the isomers *Z/E* on biological activity. The simplest and the most often naturally occurring  $\alpha,\beta$ -dehydroamino acid is dehydrobutyrine, 2-amino-but-2-enic acid [2]. In peptide synthesis, dehydrophenylalanine (2-amino-3-phenylpropenoic acid,  $\Delta$ Phe) (Figure 1) is the most often used, mainly the isomer *Z*, but the isomer *E* can be easily obtained through photochemical inversion [3]. The example of tentoxine and isotentoxine shows that both isomers have different influence on peptide conformation and in consequence on bioactivity. Literature survey shows that (*Z*)- $\Delta$ Phe adopt almost exclusively helical conformations  $\alpha/-\alpha$  with the values of torsion angles  $\phi$  and  $\psi$  in the range of  $-61^\circ$ ,  $-21^\circ$  for  $\alpha$  and  $61^\circ$ ,  $21^\circ$  for  $-\alpha$  and. Such symmetry related conformations are typical for the  $\alpha,\beta$ -dehydroamino acids, which do not reveal optical stereoisomers. The scarce literature data for (*E*)- $\Delta$ Phe reveals that it does not show similar property.

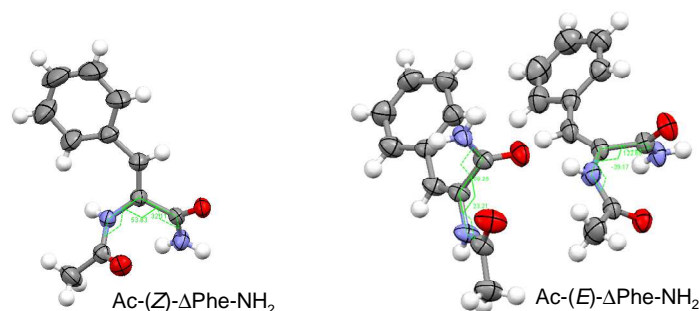


**Fig. 1.**  $\alpha,\beta$ -Dehydrophenylalanine residues, isomers *Z* and *E*.

The aim of this work is to show how the position of the phenyl ring in the side chain influence the intramolecular stabilising forces resolve within the residue as well as intermolecular interactions. The simple model compounds are the most suitable for this purpose. The effect of the other structural motifs is excluded. On the other hand, the studied structure is exposed on possible intermolecular interactions. Furthermore small size of the studied molecules enables application of theoretical methods at relatively high level of theory including simulation of the solvent effect and to obtain the crystal structures, which bring valuable information concerning both the arrangement of the structural elements in space and stabilising forces.

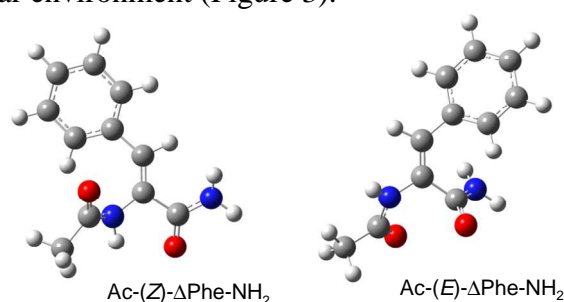
*N*-Acetyl-(*Z*)-dehydrophenylalanine amide, Ac-(*Z*)- $\Delta$ Phe-NH<sub>2</sub>, was synthesized through *N*-hydroxysuccinimide derivative. *N*-Acetyl-(*E*)-dehydrophenylalanine amide, Ac-(*E*)- $\Delta$ Phe-NH<sub>2</sub>, was obtained through photoisomerisation reaction.

The X-ray analysis reveals that Ac-(*Z*)- $\Delta$ Phe-NH<sub>2</sub> molecules adopt in the solid state the conformations  $\alpha$  ( $\phi$ ,  $\psi = -53.83^\circ$ ,  $-32.11^\circ$ ) and  $-\alpha$  ( $\phi$ ,  $\psi = 53.83^\circ$ ,  $32.11^\circ$ ), whereas Ac-(*E*)- $\Delta$ Phe-NH<sub>2</sub> molecules adopt the conformation  $\beta$  ( $\phi$ ,  $\psi = -39.17^\circ$ ,  $122.69^\circ$ ) and  $-\beta$  ( $\phi$ ,  $\psi = 23.21^\circ$ ,  $-108.29^\circ$ ) (Figure 2).



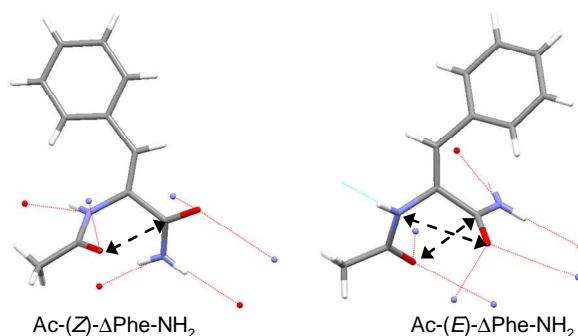
**Fig. 2.** Conformations of the studied dehydrophenylalanine compounds adopted in the crystal state.

The theoretical analysis performed at the meta-hybrid M06-2X/6-311++G(d,p) level of theory shows the adopted conformations are the lowest in energy (isomer *Z*) and the second lowest in energy (isomer *E*) in polar environment (Figure 3).



**Fig. 3.** Conformations of the studied dehydrophenylalanine compounds calculated at M06-2X/6-311++G(d,p) in water mimicking environment.

The conformational preferences depend on the balance between the intra- and intermolecular forces (Figure 4).



**Fig. 4.** Intra- and intermolecular forces stabilise the conformations  $\alpha$  and  $\beta$  of the isomers *Z* and *E* dehydrophenyl alanine.

Both adopted conformations enable to obtain stabilisation simultaneously from the N–H...O intermolecular hydrogen bonds and from the C=O ... C=O intramolecular dipole attractions. The difference in tendency toward the conformations  $\alpha$  or  $\beta$ , depends on the steric hindrance imposed by position of the phenyl ring in the side chain.

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# The impact of *N*-methylation on the $\beta$ -turn tendency in dipeptides with Aib residue

Roksana Wałęsa, Małgorzata Anna Broda

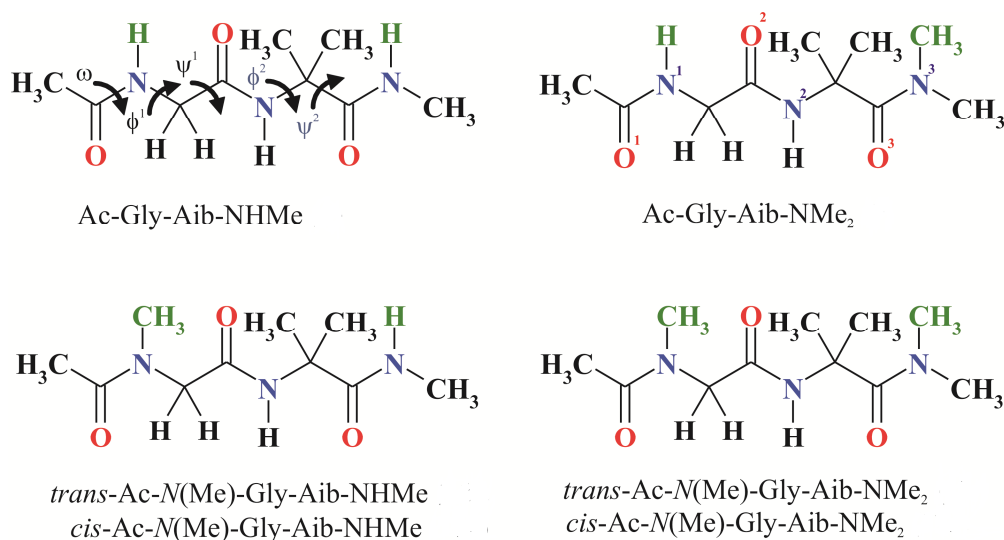
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## 1. Introduction

Beta turns are very important elements of peptides and proteins structure and have a large influence on their function [1,2]. They give rise to a sharp reversal in the polypeptide chain that result in the globular shape of the protein. Many naturally occurring peptides have been proposed to adopt turns in their bioactive conformations [3]. One of the amino acids promoting  $\beta$ -turn in peptides is Aib residue. Achiral Aib residue belongs to a group of non-protein amino acids [4]. It's somewhat alanine's derivative in which a hydrogen atom on the alpha carbon has been replaced by a methyl group.

*N*-Methylation is a structural modification, in which the amide proton is replaced by *N*-methyl group. 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 [5]. Besides, the lack of an amide hydrogen atom (one or more) prevents the formation of intramolecular hydrogen bonds, limits the conformational freedom of the side and main peptide chain and stabilizes specific, well-defined secondary structures including  $\beta$ -turn conformations.

In this work, the tendency to adopt  $\beta$ -turn conformation by model dipeptides with Aib residue in the gas phase and in solution is investigated by theoretical methods (**Figure 1**). We pay special attention to the influence of *N*-methylation on  $\beta$ -turn stability.



**Figure 1.** Chemical structures of studied dipeptides.

## 2. Results

Surprisingly, our calculations predict, that tendency to adopt  $\beta$ -turn conformation is similar in the case of Ac-Gly-Aib-NHMe and Ac-Gly-Aib-NMe<sub>2</sub>, although it should be significantly reduced due to *C*-terminal tertiary amide bond preventing the 4  $\rightarrow$  1 hydrogen

bonding. In the gas phase the  $\beta$ -turn conformations for Ac-Gly-Aib-NHMe and for Ac-Gly-Aib-NMe<sub>2</sub> are high in energy but in water became global minimum.

Slightly different preferences were observed for Ac-*N*(Me)-Gly-Aib-NHMe and Ac-*N*(Me)-Gly-Aib-NMe<sub>2</sub>. Especially, in the gas phase the tendency to adopt  $\beta$ -turn conformations is much weaker for Ac-*N*(Me)-Gly-Aib-NMe<sub>2</sub>. C-Terminal amide bond in Ac-*N*(Me)-Gly-Aib-NMe<sub>2</sub> reduces the stability of  $\beta$ -turn conformation.

On the other hand, we observed, that the presence of the tertiary amide groups both at the *N*- and *C*-terminal in Ac-*N*(Me)-Gly-Aib-NMe<sub>2</sub> significantly increases the population of the *cis* *N*-terminal amide bond. Moreover, polar environment increases the tendency of methylated peptide bond in studied compounds to adopt the *cis* configuration, because but in water the energies of *trans* and *cis* conformers are almost equal.

### 3. Acknowledgments

Roksana Wałęsa is a recipient of a Ph.D. scholarship under a project funded by the European Social Fund. Calculations were carried out in Wrocław Centre for Networking and Supercomputing (<http://www.wcss.wroc.pl>), and in the Academic Computer Centre CYFRONET, AGH, Kraków, grant MEiN/SGI3700/UOpolski/063/2006.

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# PAAD: A PLATFORM FOR ANALYSIS AND ARCHIVIZATION OF SCIENTIFIC DATA

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**Keywords:** interactive scientific computing, large-scale scientific data analysis, high-performance computing

In many areas of research there are increasing demands for processing large amounts of data in combination with high performance computing. Usually the data generated during the research should remain available for a longer time, sometimes even indefinitely, e.g., for further use or as an archival record. In order to meet such needs it is therefore necessary to augment the HPC infrastructure with the appropriate storage facilities and software. Another important factor is the increasing demand for interactivity in scientific computing instead of the traditional batch-oriented approach.

In the present contribution we want show from a bird's-eye perspective the PAAD platform being developed about a year at the University of Silesia and aimed at implementation of good management practices to the process of analysis and archivization of data generated during research in various disciplines. The platform will provide a wide range of software tools used in computational physics and chemistry, material science, biology and earth sciences, with emphasis on performing all the operations online whenever possible.

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# **Theoretical studies of mechanism of Traditional Chinese medicine: Astragalus membranaceus**

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2. Theoretical Chemistry Group, Faculty of Chemistry, Tsinghua University, China

Astragalus membranaceus is a famous Chinese medicine which has pharmacological effects on Hypertension and Ischemic cardiopathy. Scientists used different methods to explain its mechanism. We have focused on its theoretical studies of mechanism at molecular level, and compared properties such as molecular structures, bond length, atomic charges, bond orders, hybrid orbital, HOMO-LUMO gap and IR spectrum between Astragaloside IV which is the most important compound to qualify and quantify Astragalus membranaceus and Digoxin because they have same pharmacological effects. After comparing these two compounds we found that their properties are almost the same. Digoxin is a representative of cardiac glycosides which is an well-known anti-heart medicine all over the world. And functional mechanism of cardiac glycosides make the concentration of  $\text{Ca}^{2+}$  increase because it restrains  $\text{Na}^+\text{-K}^+\text{-ATP}$  enzyme of pericardium. We infer that Astragaloside IV has the same mechanism as Digoxin.

## CYANOBACTERIA AS AN ATTRACTIVE SOURCE OF PHOTOSYNTHETIC PIGMENTS AND VALUABLE BIOACTIVE NATURAL COMPOUNDS

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**Keywords:** cyanobacteria; photosynthetic pigments; carotenoids; phycobilins; flavonoids

Cyanobacteria (blue green algae) are widely distributed, extremely diverse morphologically and metabolically, and phylogenetic unique group of Gram-negative oxygenic photosynthetic prokaryotes. These microorganisms possess several advantages as hosts for biotechnological applications, such as rapid biomass increase, ease and low costs of maintaining culture, ability to exhibit a wide range of tolerance to multiple environmental factors, diversity of their metabolism and production of many secondary metabolites that possessing biological activity. The enormous biodiversity, and the consequent variability in the respective biochemical composition make cyanobacteria a new and rich sources of many valuable compounds, including important bioactive and biotechnologically relevant chemicals. Therefore the cultivations of these microorganisms are a promising resources for many novel chemically and biologically active molecules and compounds of high commercial value [1]. The range of biological activity of secondary metabolites isolated from cyanobacteria includes among others: antibacterial, antifungal, antiviral, anti-inflammatory, antialgal, antiprotozoal, anticancer and antioxidant activities [2] that are of pharmaceutical and agricultural significance, whereas cyanobacterial pigments [3] and phytonutrients – flavonoids [4], are known for their biotechnological purposes. Two important groups of cyanobacterial pigments, phycobiliproteins and carotenoids, are extensively used in bioindustry and possess high commercial value [3]. Thus interesting aspect of this attempt is the fact that the nature of the chemicals produced by these photosynthetic microorganisms can be influenced by changing the conditions of cultivation.

In our study, several strains of halophilic and freshwater cyanobacteria were selected considering the production of mentioned substances using thin layer chromatography and gas chromatography coupled with mass spectrometry or flame ionization detector. Obtained results indicated that halophilic strains: *Spirulina platensis*, *Arthrospira maxima* and *Arthrospira fusiformis* were abundant source of the compounds of interest.

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