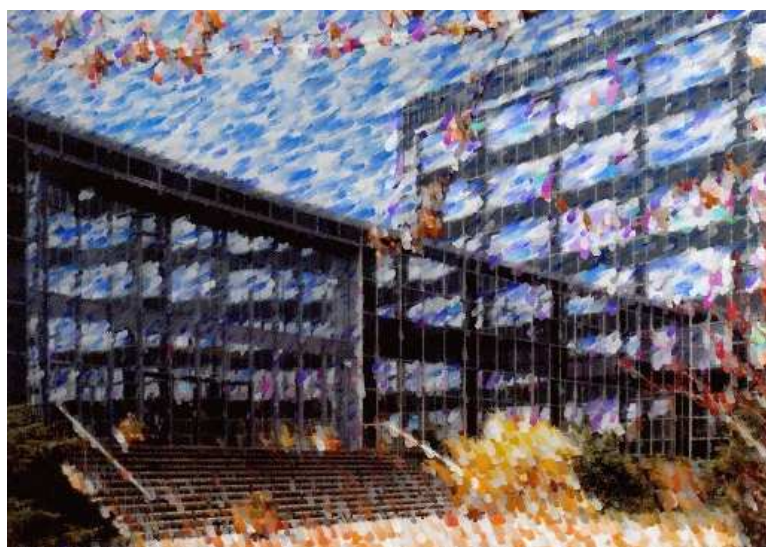
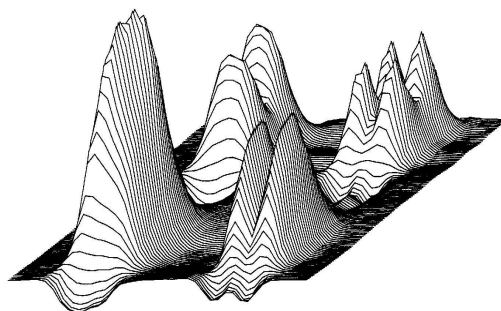


2. Workshop on Solid-State NMR and Computational Methods

OCTOBER 20, 2006 PRAGUE



Institute of Macromolecular Chemistry AS CR
Heyrovského nám. 2
162 06 Praha 6



Introduction

Joint Laboratory Of Solid-State NMR

of the Institute of Macromolecular Chemistry Academy of Sciences of the Czech Republic (IMC AS CR) and of the Jaroslav Heyrovský Institute of Physical Chemistry of Academy of Sciences of the Czech Republic (JHIPC AS CR)

organizes on

Friday October 20, 2006

The Second Workshop on Solid-State NMR and Computational Methods

in

Lecture Hall "A"

of the

**Institute of Macromolecular Chemistry (IMC)
of the Academy of Sciences of the Czech Republic,
Heyrovsky Sq. 2, Prague**

Information

Last November in our Institute an informal workshop was held presenting the ongoing investigations and research ideas of several groups involved in solid-state NMR measurements and simulations. We would like to go on with the discussions and also introduce the research devoted to the vastly important subject of the polymorphism of organic compounds, where the solid-state NMR and computations are becoming increasingly useful.

Not only NMR spectroscopists and structural chemists, but also other interested scientists and students are cordially invited.

There is no registration fee and the number of participants is not limited.

However, meals and accommodation are not provided.

Program

Schedule (as extensive discussions are expected, only approximate starting/ending times of the lectures are given):

9:00 am	Welcome Coffee
9:25 am	Opening
9:30 am - 10:00 am	Alexandr Jegorov , <i>TEVA Pharmaceuticals, CR</i> , "Polymorphism and its Role in Bioavailability of Active Pharmaceutical Ingredients"
10:00 am - 10:30 am	Jiří Czernek , <i>IMC Prague, CR</i> , "Perindopril Erbumine"
10:30 am - 11:15 am	Jiří Brus , <i>IMC Prague, CR</i> , "Polymorphism in Pharmaceutical Solids, Structure and Dynamics: Toward Powder NMR Crystallography"
11:15 am - 12:30 pm	Lunch Break
12:30 pm - 1:00 pm	A tour of solid-state NMR and computational facilities at IMC
1:00 pm - 1:45 pm	Martin Nausner , <i>Johannes Kepler University Linz, Austria</i> , "Applications of the ONIOM Model to Molecular Clusters"
1:45 pm - 2:30 pm	Zdenek Tosner , <i>Charles University, Prague, CR</i> , "Optimal Control in Design of New NMR Experiments in Solids"
2:30 pm - 3:00 pm	Coffee Break
3:00 pm - 3:30 pm	Jan Lang , <i>Charles University, Prague, CR</i> , "NMR Relaxation as a Tool to Study Arrays of Hydrogen Bonds"
3:30 pm - 4:00 pm	Radek Marek , <i>Masaryk University Brno, CR</i> , "Chemical Shift Tensors in Purines"
4:15 pm	Closing remarks
4:30 pm	A walk to the Hvězda Folly (weather permitted)
5:30 pm	Round Table Discussions

Transportation

The Institute of Macromolecular Chemistry is situated in the western suburb of Prague, called "Petriny".



If you travel from abroad by air plane, by train, or by coach you will probably arrive at one of the following points:

1. Airport Praha Ruzyně
2. Railway station Praha hlavní nádraží
3. Railway station Praha-Holešovice (trains Berlin - Wien/Budapest)
4. Central coach station Praha-Florenc

From them, you may use *Prague integrated transport (PIT). The tram and bus stops Petriny, located in front of the Institute, are terminals of the tram and bus lines:

Tram

- 1** Vychovatelna - Palmovka - Nádraží Holešovice - Hradčanská - Petřiny
2 Červený Vrch - Dejvická - Petřiny
18 Vozovna Pankrác - Pražského povstání - Karlovo náměstí - Národní třída - Staroměstská - Malostranská - Hradčanská - Petřiny

Bus

- 179** Letiště Ruzyně - Petřiny - Nové Butovice
184 Nové Butovice - Petřiny
191 Letiště Ruzyně - Petřiny - Nové Butovice

*PIT consists of public transport services in Prague (Metro, trams, funicular to Petřín, city buses), suburban bus service (lines of series 300 and 400) and railway service (only 2nd class passenger and fast trains and selected express trains - specified in timetables of the Czech Railways) in Prague and suburban regions.

The most common tickets are:

	Tickets	
	Transfer	Non-transfer
Adult persons over 15 years	20,- CZK	14,- CZK
Children from 6 up to 15 years inclusive	10,- CZK	7,- CZK

Transfer tickets. Tickets for three fare zones can be used 75 minutes from validation. On working days from 08.00 PM to 05.00 AM and on Saturdays and Sundays round the clock such tickets can be used 90 minutes from validation.

Non-transfer tickets. Apply to trams and buses 20 minutes allowing no change. On the Metro such tickets are valid for the distance of 5 stations from the station of validation (not including the station of validation) allowing to change between the lines A,B,C, but no longer than 30 minutes. These tickets do not apply to night routes and funicular railway. Tickets are available at newspaper stands and tobacco shops, at hotel reception desks, in restaurants, at railway stations, at the airport, in slot machines at some stops, etc. The Metro runs from 5 a.m. till midnight.

Additional ticket sale from bus drivers

- Adult persons over 15 years 25,- CZK
Children from 6 up to 15 years inclusive 15,- CZK

Tickets must be purchased in advance and punched inside the tram or bus or before passing the gates of the Metro.

Contacts

Mr. Jiří Brus - Head of the Joint Laboratory of Solid-State NMR

Mr. Jiří Czernek - Chairman of the Workshop

	email	phone	GSM
Jiří Brus	brus@imc.cas.cz	+420-296809380	+420-723885144
Jiří Czernek	czernek@imc.cas.cz	+420-296809290	+420-776600179

Úplná Adresa

Ústav Makromolekulární chemie
AV ČR
Heyrovského nám.2
162 06 Praha 6 - Břevnov
Česká republika

Full Address

Institute of Macromolecular Chemistry
AS CR
Heyrovsky Sq. 2
162 06 Praha 6 - Brevnov
Czech Republic