XVII International Conference
"Horizons in Hydrogen Bond Research"

and Graduate Student Research School on
"Hydrogen Bonding and Proton Transfer"

PROGRAM

LIST OF PARTICIPANTS

September 1 - 8
2007
Saint-Petersburg, Russia

Organized by:
V.A. Fock Institute of Physics
St. Petersburg State University

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Aleksey A**. Tsyganenko** St. Petersburg University, St. Petersburg

Welcome!

It is a great pleasure to welcome all of you to St. Petersburg on a coast of the Finnish Bay in Repino. I hope that your participation in Horizons 2007 will be enjoyable, useful and memorable.

I have been greatly helped by the International Advisory Board, Program and Organizing Committee and Local Organizing Committee.
With the great pleasure I would like to thank for the help Institute of Physics of St. Petersburg University, The Russian Foundation for Basic Research, Deutsche Forschungsgemeinschaft (DFG) and company „Monomax“

Konstantin Tokhadze (chair of Horizons 2007)

Conference site
www.onlinereg.ru/Hbond2007

Conference address:
St. Petersburg, Repino, Primorskoye shosse **427**

Telephone: (8-904-641-19-74) for contact

If you have any questions or need any help please **feel free to contact** any member of the local organizing committee (they will be identifiable by a badge of a **different colour**) at any time. You may as well ask at the hotel's reception desk.

THIS PROGRAM includes: the **schedule** of conference and poster sessions (**pp**.**6 - 16**), the late **abstracts (pp.17-22)**, the list of participants (**pp.23-32**) and some **general information (pp. 1-5)**, including the **elementary plan of transfer** from St. Petersburg to Repino

The conference will start with morning session on **Monday. September 3, Registration**

September 1 and **September 2** from **10:00 to 19:00**

Meals
The breakfasts will be served between **8:30** and **10:30** each morning
The lunch – between **13:30** and **15:00**
The dinner – between **18:00** and **19:30**

Get-together party and dinner will begin at 20:00 on Sunday, **September 2**

Conference dinner
Conference dinner is planned on Friday, **September 7,** after our excursion to Peterhof

Posters
We plan to carry out two poster sessions, on Monday, **September 3** and Tuesday, **September 4** (15.30-16.50). Each poster will carry an identification number (see pages 11-16 in this program) on the top left or right corner. Please remove your poster the next morning after your presentation.

International Advisory Board
The advisory board will meet on **September 6**

General Information

Time difference
Time in St. Petersburg differs from Central European time on two hours

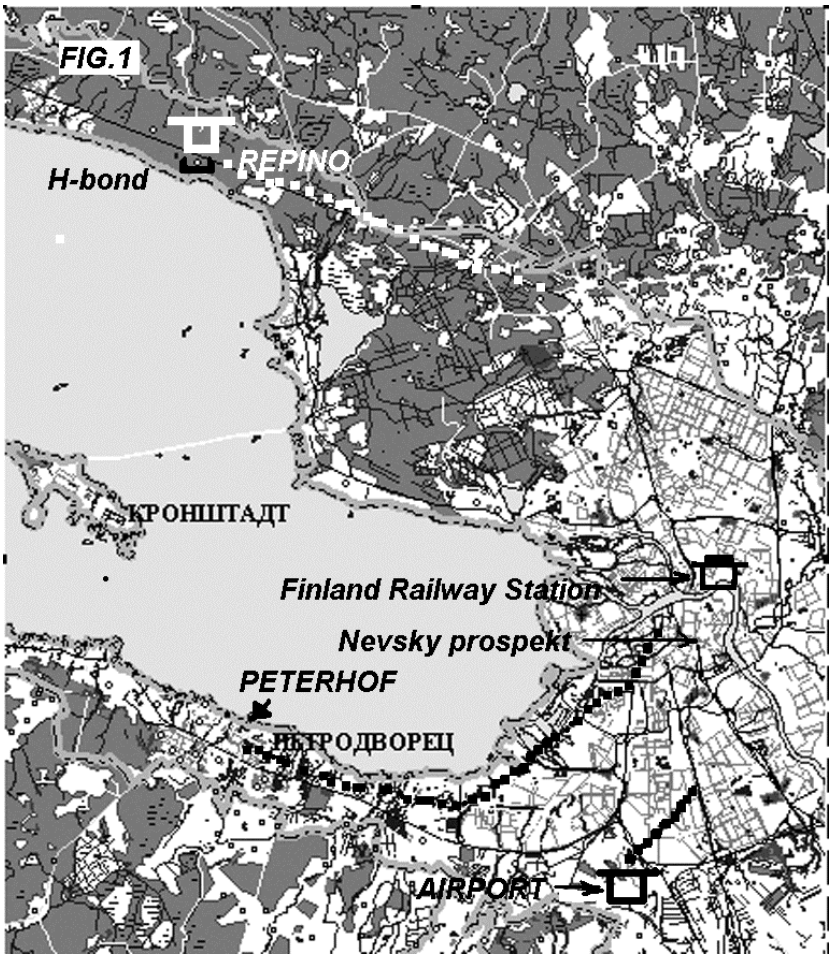
Currency and Exchange rates
The Russia currency is Rouble (**Roub**). At the moment one **Euro (€)** is equivalent to approx. **Roub** 34.8, one **US ($)** is equivalent to **Roub** 25.5

***Attenion*!!!** All payments in shops and transport can be made only in roubles. The conference participants can convert money to roubles at currency exchange offices or at banks. Of course it is possible to use credit card and cash points.

Transport

The ticket's price is **14** roubles per one-way trip for all kinds of municipal transport (**Metro**, **Bus, Tramway and Trolley bus**) in St. Petersburg.

The XVII-th Conference will be held in small town **Repino** located in 40 kms from the centre (**Nevsky prospect**) of St. Petersburg on a coast of the Finnish Bay. The location of **Repino** in relation to the centre of St. Petersburg and airport "**Pulkovo**" is shown in Fig.1. From this figure one can see also the position of **Peterhof,** where excursion is planned on Friday September 7 and where will be a conference dinner.



Dear participants of the Conference, you can get to us as follows:

1. From the railway station "**Finlyandskii voksal**" (metrio station "**Lenin's square**") by the train to station "Repino" in the direction to Zelenogorsk or Viborg (*The approximate time table for train from Petersburg:* ***5****.51, 56,* ***6****.40, 58,* ***7****.19,* ***8****.10,* ***8****.30,* ***9****.22,* ***9****.44,* ***10****.15,* ***10****.54,* ***11****.15,* ***11****.45,* ***12****.04,* ***12****.26,* ***13****.05,* ***13****.40,* ***14****.26,* ***14****.54,* ***15****.02,* ***15****.15,* ***16****.05,* ***16.****30,* ***16****.43,* ***16****.54,* ***17****.05,* ***17****.20,* ***17****.55,* ***18****.15,* ***18****.40,* ***19****.06,* ***19****.35,* ***20****.14,* ***21****.07,* ***21****.53,* ***22.****45,* ***23****.46)*

2. From the railway station "**Finlyandskii voksal**" (metrio station "**Lenin's square**") by commercial bus №. **K-400** to "Baltiets" (bus stop on demand),

3. From the metro station "**Chernaya rechka**" by bus №. **211** to the bus stop "Repino – centre", operating time from 6 till 23.40, an interval is about **20** min.

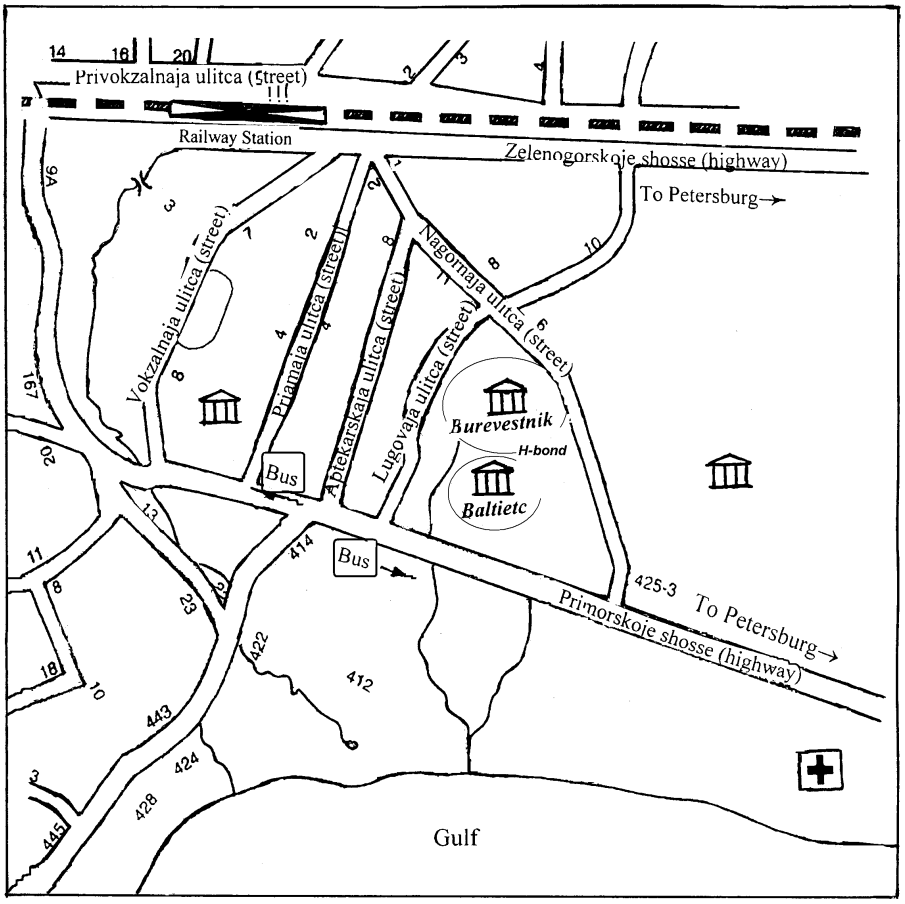
4. From the metro station **"Staraya derevnya**" by commercial bus №. **305** to "Baltietc" (bus stop on demand), operating time from 7 till 22.00, an interval is **20** min

DIAGRAM of METRO LINES and STATIONS

5. From the metro station "**Prospekt prosvechsheniya**" by commercial bus **№. 680** to "Baltiets" (bus stop on demand), operating time from 7 till 22.00, an interval is about **20** min.

The map of Repino in a vicinity of Hotels "Baltietc" and "Burevestnik"

Repino



PROGRAM

Graduate Student Research School

Saturday, 1 September (14.20-18.45) - **Sunday, 2 September (**9.30-19.35)

Horizons in Hydrogen Bond Research

Sunday, 2 September

11.00 - 19.00 Registration
20.00 - **Welcome drink**

Monday, 3 September

9.30 – 9.50	L. Sobczyk, Wroclaw	**Georg Zundel Memory Lecture**
9.50 - 10.10	H. Ratajczak, Wroclaw	**Camille Sandorfy Memory Lecture**

Session 1: **Coupled hydrogen bonds**			Discussion leader**: A. Koll,** Wroclaw
10.20 -11.00	**L1**	M. Suhm, Göttingen	Vibrational spectra of proton transfer models in supersonic jets
11.00-11.20	**O1**	P. Wolschann, Vienna	Molecular calculations on hydrogen bonds in cyclodextrins
11.20 -11.40	**O2**	T. Zeuch, Göttingen	Experimental and theoretical study of the microsolvation of sodium atoms in methanol clusters: differences and similarities to sodium/water and sodium/ ammonia
Coffee break			
12.00-12.40	**L2**	J. Waluk, Warsaw	Role of vibrations in photoinduced tautomerization
12.40 -13.00	**O5**	W. Werncke, Berlin	Mode-selective O-H stretching excitation in an intramolecular hydrogen bond studied by ultrafast vibrational spectroscopy
13.00 -13.20	**O4**	M. Kijak, Warsaw	Excited state proton transfer in supersonic-jet-isolated 2-(2 pyridyl) pyrrole
13.20 -13.40	**O3**	Z. Mielke, Wroclaw	The effect of molecular complexation on the photochemistry of glyoxal
13.40-14.00	**O6**	A.A. Levin, Moscow	Deuteration-induced structural phase transition versus quantum paraelectric behavior: quantum chemical modeling of H/D-bonded materials
14.00 -15.30		**Lunch**	
15.30 -16.50		**Poster session 1**	**P1.1- P1.40 S1 – S6 S18 – S21**
Coffee break			

Session 2: **Unconventional hydrogen bonds** Discussion leader: **L. Epstein,** Moscow			
17.00 -17.40	**L3**	N. Belkova, Moscow	Conformities of proton transfer via unconventional hydrogen bonds
17.40- 18.00	**O7**	L. Sobczyk, Wroclaw	The effects of conventional and unconventional hydrogen bonds on dynamics of methyl groups in complexes of tetra- and dimethylpyrazine
18.00 -18.20	**O8**	R. Rivelino, Salvador	Lewis acid-base interactions in weakly bound formaldehyde complexes with CO_2, HCN, and FCN: considerations on the cooperative H-bonding effects
18.20 -18.40	**O9**	J. Sadlej, Warsaw	Characterisation of dihydrogen-bonded D-H...H-A complexes on the basis of spectroscopic parameters
18.40 -19.00	**O10**	V.D. Maiorov, Moscow	The effect of 1,1,2,2-tetrachloroethane on the equilibrium between uncharged and ionic complexes in solutions of acids
Dinner			
20.00- 20.40	**L4**	E. Kryachko, Liege	Nonconventional hydrogen bonds with gold
20.40- 21.00	**O11**	A. Koll, Wroclaw	Self-assembling of molecules containing the 2-aminopyridine unit in non polar solvents
21.00- 21.20	**O12**	I. Natkaniec, Dubna	DFT studies of hydrogen bonded molecular clusters and vibrational spectroscopy of 2,2-dimethyl-1-butanol and 2,3-dimethyl-2-butanol

Tuesday, 4 September

Session 3: **Single hydrogen bonds** Discussion leader: **A. J. Barnes,** Salford			
9.30 - 10.10	**L5**	L. Khriachtchev, Helsinki	Rotational isomers of small molecules in noble-gas solids: From monomers to hydrogen-bonded complexes
10.10-10.50	**L6**	P.E. Hansen, Roskilde	Transmission of isotope effects via hydrogen bonds as studied by NMR
10.50-11.10	**O13**	P.M. Tolstoy, Berlin	Geometries of OHO hydrogen bonds probed by H/D isotope effects on nearest carbon chemical shifts
11.10-11.30	**O14**	S.K. Ignatov, Nizhny Novgorod	Potential energy surfaces of hydrogen-bonded complexes $H_2O{\cdot}O_3$ and $H_2O{\cdot}SO_2$ and their thermodynamic properties with explicit accounting of rovibrational contributions
Coffee break			

11.50 -12.30	**L7**	M.V. Vener, Moscow	Towards the quantitative description of the H-bonds in the alanine-based secondary structures. The IR frequency shifts and electron-density features
12.30 -12.50	**O15**	S. Melandri, Bologna	How ammonia participates in hydrogen bonding
12.50 -13.10	**O16**	P. Asselin, Paris	Vibrational dynamics of hydrogen bonded complexes : FTIR spectroscopy and ab initio theory
13.10 -13.30	**O17**	W. Herrebout, Antwerp	A cryosolution FTIR study of the C-H(D)...O hydrogen bonded complexes between dimethyl ether(-D_6) and halothane(-D_1)
13.30 -13.50	**O18**	S. Coussan, Marseille	UV and IR photoisomerisation in cryogenic matrices of *intra* and *inter*molecularly H-bonded molecules and aggregates
Lunch			
15.30 -16.50		**Poster session 2**	**P2. 1 – P2. 35, S7 – S17**
Coffee break			
Session 4: **Hydrogen bonds in solids** Discussion leader**: I. Shenderovich,** Berlin			
17.00 -17.40	**L8**	T. Krygowski, Warsaw	Long distance consequences of H-bonding
17.40 -18.00	**O20**	J.Blazejowski, Gdansk	Hydrogen bonded complexes and inter-molecular interactions in molecular crystals of acridine derivatives and flavonols
18.00 -18.20	**O21**	H. Ratajczak, Wroclaw	On the role of the hydrogen bond in nonlinear optical properties of molecular hydrogen-bonded crystals
18.20 -19.00	**L9**	I. Olovsson**,** Uppsala	The role of the lone pairs in hydrogen bonding
Dinner			
20.00-20.20	**O19**	A.O. Borissova, Moscow	The role of cooperative effects of H-bonding in molecular crystals
20.20- 20.40	**O22**	M. Szafran, Poznan	Prototropic equilibrium between 1-h-2-oxo-pyrido[2,1-b][3,4]dihydropyrimidinium chloride and 3-(2-aminopyridinium) propionate hydrochloride studied by X-ray, FTIR, Raman, NMR and ab initio methods
20.40- 21.00	**O23**	J. Zachara Hore-glad, Warsaw	Extension of the Clar rule on pi-electron systems with H- or Li-bonding
21.00- 21.30	**L18**	M.R. Johnson, Grenoble	Inter-molecular hydrogen bonds; from temperature-driven proton transfer in molecular crystals to DNA

Wednesday, 5 September - Cultural program

Thursday, 6 September

Session 5: **Hydrogen bonds of biological interest** Discussion leader**: P. E. Hansen,** Roskilde			
9.30 - 10.10	**L10**	H.H. Limbach**,** Berlin	NMR studies of H-bonding
10.10- 10.50	**L11**	W. Saenger, Berlin	Functional role of C-H···O hydrogen bonds between transmembrane a-helices in photosystem I
10.50-11.10	**O24**	P. Storoniak, Gdansk	Thermodynamics of hydrogen transfer within the neutral radicals of nucleotides. A proposal of DNA strand break formation induced by an excess electron
11.10-11.30	**O25**	Z. Dega-Szafran, Poznan	New hydrogen-bonded complexes of para-hydroxybenzoic acid with zwitterionic compounds
Coffee break			
12.00 -12.40	**L19**	K. Gerwert, Bochum	Proteins in Action: Monitored by TR (time-resolved) FTIR spectroscopy
12.40 -13.00	**O26**	A.V. Bochenkova, Moscow	Role of hydrogen bonding in photo-absorption of biological chromophores
13.00 -13.20	**O27**	R.A. Skochilov, Kazan	Self- and heteroassociates of cumyl hydroperoxide: FTIR-spectroscopy, chemometrics (factor analysis) and quantum chemical calculations
13.20 -13.40	**O28**	M. Vantsyan, Moscow	Molecular architecture of oligoaminoacid derivatives assemblies
13.40 -14.00	**O29**	J. Graton, Nantes	Hydrogen-bond properties of two n AChRs allosteric modulators: galantha-mine and codeine probed by FTIR spectroscopy and theoretical calculations
Lunch			
Session 6: **Hydrogen bonds in interfaces** Discussion Leader **A.A. Tsyganenko**, St. Petersburg			
15.30 -16.10	**L12**	C. Otero Arean**,** Palma de Mallorca	Dinitrogen and carbon monoxide hydrogen bonding in protonic zeolites: studies from variable-temperature infrared spectroscopy
16.10 -16.30	**O30**	A.V. Rudakova, St.Petersburg	FTIR study of processes on disperse ice surface
16.30 -15.50	**O31**	N.K. Moroz, Novosibirsk	NMR study of proton transfer in microporous crystals
Coffee break			

17.10 -17.50	**L13**	S. Shaikhutdinov**,** Berlin	Adsorption of water on well defined oxide surfaces
17.50 -18.20	**O32**	N. Perez-Hernandez, Berlin	Solid state NMR description of dynamics in porous self-assembly structured via hydrogen bonds and containing water clusters
18.20 -19.00	**L14**	J. Sodeau, Cork	Novel atmospheric chemistry driven by "micropockets" and Quasi Liquid Layer (QLL) in water-ice
Dinner			
20.00- 21.00	**Round table**		

Friday, 7 September

Session 7: **Water and aqueous solutions** Discussion leader**: M. – C. Bellissent-Funel,** Gif-sur- Yvette			
9.00 – 9.40	**L15**	Y. Marechal, Grenoble	From physics to biology: a journey through science, accompanying the hydrogen bond and the water molecule
9.40-10.20	**L16**	S. Bratos, Paris. ***(in memoriam A. Novak)***	Temporal evolution of the structure of hydrogen bonds in water at subpico-second time scales
10.20-10.40	**O33**	S. Canuto, Sao Paulo	Hydrogen bond interaction between a probe molecule and normal and supercritical water. Influence on spectroscopic properties
10.40 -11.10	**L17**	M.-C. Bellissent-Funel**,** Gif-sur-Yvette	Hydrogen bonding in supercritical water
Lunch			
Excursion to Peterhof			
Conference dinner in Peterhof			

POSTERS

Monday, 3 September, 15.30 - 16.50

Poster session 1		
S18	Albrecht M., Rice C.A., Suhm M.A.	FTIR spectroscopy of strongly bound hydrogen-bonded clusters
S19	Chwaleba D., Ilczyszyn M., Ciunik Z.	Relation between hydrogen bond network and crystal structure of sarcosine – p-toluen-esulfonate (1:1)
S20	Dauster I., Suhm M.A., Buck U., Zeuch T.	How much can the ionization potential of sodium be influenced by methanol solvation?
S21	Turkmen I.R.	A Modified Statistical Thermodynamic Model of Liquid Water and the Kinetics of Phase Transition in Supercooled Liquid Water
P1. 1	Borowiak T., Dutkiewicz G., Sobiak S., Rozanski J.	Supramolecular structures of N,N-bis(2-hydroxyethylamidine) derivatives: the role of hydrogen bonds
P1. 2	Puszko A.P., Gurzycski J.G., Chmurzycski L.	Basicity of di-substituted 4-nitropyridine derivatives in polar non-aqueous media studied by potentiometry
P1. 3	Holderna-Natkaniec K., Natkaniec I., Mikuli E., Jakubas R., Swiergiel J.	The dynamics of 4-aminopyridine complexes with different anions
P1. 4	Leyva V., Corral I., Gonzalez L.	Hydrogen transfer in ortho-Nitrobenzaldehyde. A Theoretical Study
P1. 5	Lu K.-L.	Bamboo-like water pipes consisting of alternate octameric water cube and $(H_2O)_{22}$-cluster encapsulated in 3d-4f metal-organic networks
P1. 6	Majewska P., Rospenk M., Czarnik-Matusewicz B., Sobczyk L.	Polarized IR spectra of resonance assisted hydrogen bond (RAHB) in 2-hydroxyazobenzenes
P1. 7	Melikova S.M., Rutkowski K.S., Shchepkin D.N., Shapkina O., Koll A., Janski J.	FTIR and ab initio studies of anharmonic coupling in the spectrum of acetic acid dimer
P1. 8	Melikova S.M., Rutkowski K.S., Shchepkin D.N.,Baskin A.I., Lipkowski P., Koll A.	Anharmonic effects in the weak OC…HCl complex
P1. 9	Sedov I.A., Solomonov B.N.	Determining the Gibbs energies of solute-solvent hydrogen bonding in infinitely diluted solutions of nonelectrolytes using a novel empirical method
P1. 10	Golubev N.S., Detering C., Tolstoy P.M., Limbach H.-H., Denisov G.S.	Low-temperature NMR spectra of a strongly hydrogen bonded anionic cluster, CNH...F^-, in solution

P1. 12	Wroblewska A., Sobolewski A., Domcke W.	The nature of ESIPT in (di)flavonols - computational studies
P1. 13	Varfolomeev M.A., Abaidullina D.I., Solomonov B.N.	Quantitative parameters of H-bond cooperativity in complexes of alcohols and amines in solution
P1. 14	Varfolomeev M.A., Solomonov B.N.	Solvent effects on stretching vibration frequencies in IR-spectrums. Assessment of H-bond cooperativity
P1. 15	Buturlimova M.V., Zelikina G.Ya., Kiseleva M.B., Nesterov A.S.	Role of intermolecular interactions in the formation of the absorption spectrum of mercury in organic solvents
P1. 16	Herrebout W., Hauchecorne D., Szostak R., van der Veken B.J.	A cryosolution FTIR study of the C-X...O halogen bonded the C-H...O hydrogen bonded com-plexes $(CH_3)_2O{\cdot}CF_3Cl$, $(CH_3)_2O{\cdot}CF_3Br$, $(CH_3)_2O{\cdot}(CF_3Br)_2$, $(CH_3)_2O{\cdot}CF_3I$ and $(CH_3)_2O{\cdot}CF_3H$
P1. 17	Kryachko E.S.	On Blue-Shifted Hydrogen Bonds
P1. 18	Kolomiitsova T.D., Shchepkin D.N., Tokhadze I.K. , Tokhadze K.G.	Inert matrix effect on absorption spectra of weak comlexes
P1. 19	Wang C.-C.	3D Extended Architectures of Metal-bpma Complexes via Metal-ligand bonds, hydrogen bonds and π-π interactions (bpma = bis(pyrimidin-2-yl)amine)
P1. 20	Rutkowski K.S., Herrebout W.A., Melikova S.M., van der Veken B.J., Koll A.	FTIR and ab initio studies of blue shifted hydrogen bonded complexes. $F_2ClCH...FCD_3$ and $Cl_2FCH...FCD_3$ in liquefied krypton
P1. 21	Rutkowski K.S., Melikova S.M., Rodziewicz P., Herrebout W.A., Reznikov A.A., van der Veken B.J., Koll A.	Solvent effect on the blue shifted weakly H-bound $F_3CH...FCD_3$ complex
S1	Perez-Hernandez G., Gonzalez-Vazquez J., Gonzalez L	FHF^-: Potential Energy Surface, Vibrational Eigenfunctions and Infrared Spectrum of a Strong Hydrogen Bond. A Theoretical Three-Dimensional Time-Dependent Study
S3	Martin I., Langer J., Illenberger E.	Chemical Reactions in Fluorinated Carboxylic Acid Esters Induced by Low Energy Electrons
S6	Ullah S., Hansen P.E., Kamounah F.	β-hydroxyesters, tautomerism or not studied by deuterium isotope effects on ^{13}C chemical shifts and DFT calculations
P1. 22	Asfin R.E.	Study of the ν(OH) band in the IR spectra of hydrogen bonded dimers of phosphinic acids at T from 600 K down to 12 K in the gas phase, solutions, matrix isolation, and solid state
P1. 23	Asselin P., Soulard P., Madebine B., Alikhani E.M.	Gas phase infrared spectroscopy of the reactive hydrogen bonded complex C_4H_4O-HCl

P1. 24	Bil A., Latajka Z.	On the anharmonicity of the H-X (X=F,Cl,Br) stretching mode in the HOO-HX, HOF-HX and H_2O_2-HX hydrogen bonded complexes. Ab initio study
P1. 25	Bober K., Latajka Z.	Towards a better understanding of ionic liquids anions – CO_2 interactions
P1. 26	Bulychev V.P., Gromova E.I., Tokhadze K.G.	Experimental and nonempirical theoretical studies of the H-F stretching band in the absorption spectrum of $(CH_3)_2O$…HF in the gas phase
P1. 27	Bureiko S.F., Golubev N.S., Kucherov S.Yu., Shurukhina A.V.	Molecular structure of H-bonded complexes of N,N-diphenylformamidine studied by IR and NMR spectroscopy and quantum chemical calculations
P1. 29	Dobrowolski M.A., Cyranski M.K., Krygowski T.M.	The interplay between the substituent effect of the bending of NO_2 group from the plane of the phenyl ring, aromaticity of the ring in 4-nitro phenol/ phenolate and H-bonding in OH…F- or O…HF
P1. 30	Guo J., Tolstoy P.M., Vasi-pov K., Koeppe B., Denisov G.S., Limbach H.-H.	Structure of Strong Hydrogen Bonds in Monoanions of Succinic Acid and Derivatives
P1. 31	Gurinov A.A., Lesnichin S., Shenderovich I.G., Limbach H.-H.	Investigation of hydrogen bonds in novel series of homoconjugated ions by low-temperature NMR spectroscopy
P1. 32	Konopacka A., Pawelka Z., Filarowski A.	Transformation of the intramolecular hydrogen bonds in methyl 2-hydroxy-3-nitrobenzoate
P1. 33	Maslov V.G., Korotkov V.I., Shenderovich I.G.	TDDFT analysis of electronic transitions in pyridine-pyridinium, quinoline-quinolinium and acridine-acridinium H-bonded complexes
P1. 34	Mucha M., Mielke Z.	Interaction between methanol and simple alpha-dicarbonyls. FTIR matrix isolation and theoretical studies
P1. 35	Orzol M., Martin I., Dabkowska J.K.I., Langer J., Illenberger E.	The formation of negative ions following 0-20eV electron impact to gas phase and condensed CH_3CH_2OH and CF_3CH_2OH
P1. 36	Szatylowicz H.	Modeling the Intermolecular H-Bonded Systems of Aniline Derivatives with Varying Energy of Interaction
P1. 37	Velino B., Melandri S., Giuliano B.M., Maris A., Ottaviani P., Caminati W., Favero L.	Weak C-H•••N hydrogen bond and internal rotation in the pyridine-trifluoromethane complex
P1. 38	Wiosna-Saiyga G., Petkova I., Thummel R.P., Sobolew-ski A., Buma W.J., Nosenko Y., Brutschy B., Waluk J.	Hydrogen-bonding-induced processes in 7-(pyridyl)indoles

P1. 39	Yang Y.	Anharmonic vibrational dynamics of small protonated complexes
P1.40	Maslov V.G., Shenderovich I.G., Korotkov V.I.	Electronic spectra of hydrogen-bonded complexes

Tuesday, 4 September, 15.30 - 16.50

Poster session 2		
P2. 1	Fedorov V.E., Tarasenko M.S., Naumov N.G., Golenkov E.O., Moroz N.K.	Evidence of strong N…H…N hydrogen bonds in coordination polymers [(H){Ln(H2O)4}{Re6S8(CN)6}]•2H2O, Ln = Yb, Lu
P2. 2	Fedorov V.E., Naumov N.G., Tarasenko M.S., Moroz N.K.	H-bonding in Octahedral Cluster Chalcocyanides
P2. 3	Moroz N.K., Golenkov E.O., Efremova O.A., Mironov Y.V., Fedorov V.E., Wang C.C.	Proton Transfer in a New Cluster Compound H[Lu(H2O)6{Re4Te4(CN)12}] 6H2O
P2. 4	Chenskaya T.B., Berg-hahn M., Kunz P., Peters W., Frank W., Klaui W.	Di(tert-butylpyrazole)zincdinitrate: Structure and Hydrogen Bonding
P2. 5	Dega-Szafran Z., Jaskolski M., Szafran M.	Hydrogen bonds in complex of nipecotic acid with para-hydroxybenzoic acid
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Delayed Abstracts

L18
INTER-MOLECULAR HYDROGEN BONDS; FROM TEMPERATURE-DRIVEN PROTON TRANSFER IN MOLECULAR CRYSTALS TO DNA

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We have combined neutron scattering and a range of numerical simulations to study hydrogen bonds in condensed matter. Two examples from a recent thesis will be presented. The first concerns proton transfer with increasing temperature in short inter-molecular hydrogen bonds [1, 2]. These bonds have unique physical and chemical properties and are thought to play a fundamental role in processes like enzymatic catalysis. By combining elastic and inelastic neutron scattering results with *ab initio*, lattice dynamics and molecular dynamics simulations, low frequency lattice modes are identified which modulate the potential energy surface of the hydrogen bond proton and drive proton transfer.
The second example concerns base-pair opening in DNA which is the fundamental physical process underlying biological processes like denaturation and transcription. We have used an emprical force field and a large scale, all-atom phonon calculation to gain insight into the base-pair opening modes and the apparent 'energy gap' between the accepted frequencies for these modes (~100 cm^{-1} or ~140 K) and the temperature of the biological processes (room temperature to 100°C) [3].

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L19
PROTEINS IN ACTION: MONITORED BY TR(TIME-RESOLVED) FTIR SPECTROSCOPY

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In the Postgenom era proteins are coming into the focus in the life sciences. Proteins are the nanomachines that perform the work in living organisms or are the receptors and mediators for external signals. By NMR and x-ray the three dimensional structural architecture of proteins are determined. In order to elucidate the function, time-resolved methods have to be applied.
FTIR difference spectroscopy can be used to monitor the reactions within proteins at the atomic level with ns time-resolution up to days [1]. In combination with site directed

mutagenesis or isotopically labelling the IR bands can be clear cut assigned to specific amino acids or ligands. This provides in combination with structural models also spatial resolution.

Based on fast scan studies on bacteriorhodopsin the key catalytic residues, asp 85 and asp 96 and their protonation kinetics are identified and summarized in a first detailed proton pump model [2]. Their structural arrangement as resolved in succeeding X-ray experiments by several groups supports this proposal. The X-ray structural model at 1.55 Å resolves in addition the oxygens of internal water molecules. Based on succeeding step scan FTIR measurements the interplay between these water molecules, a strongly hydrogen bonded water, a dangling water and a protonated water complex is elucidated in detail. It results in a controlled Grothuis proton transfer from the central proton binding site to the protein surface. [3,4]. A similar mechanism might apply in the photosynthetic reaction center [5] and the cytochrome oxydase [6]. The step scan approach is also successfully applied to the photoactive yellow protein [7].

The difference technique requires fast triggering of the protein reaction, which is easy to accomplish for the chromoproteins as described before. Progress for the investigation of non chromophoric proteins is acquired by developing a micro mixing cell for FTIR studies, allowing mixing times in the sub ms time range. This cell is used to investigate protein folding reactions [8]. Alternatively, photolabile caged compounds can be applied. Using caged GTP the GTPase mechanism of the protooncogen Ras is investigated [9,10]. Also its protein-protein interaction with the GAP protein could be studied time-resolved [11,12]. This provides a detailed insight into the catalytic mechanism by which GAP activates the GTPase by five orders of magnitude. The activation by GAP proteins is a central process in the signal transduction. In oncogenic Ras this activation process is inhibited and involved in uncontrolled cell growth. The study proves that the approach can be extended to protein-protein interactions. Recently, beside rection within the active site of a protein, also the surface change of a protein leading to protein-protein interactions is monitored (13).

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O18
UV AND IR PHOTOISOMERISATION IN CRYOGENIC MATRICES OF *INTRA* AND *INTER*MOLECULARLY H-BONDED MOLECULES AND AGGREGATES

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H-bonded *intra* and *inter*molecularly molecules and aggregates are of a prior interest because of their implications in many chemical processes especially those biochemical. In this context, UV and IR selective irradiation coupled with FTIR and UV spectroscopies have been proved to be really powerful tools in elucidating their structures. Moreover using cryogenic matrix technique allows us to study high energy isomers which are unstable at room temperature or transient species with lifetimes of few minutes or seconds. We have studied *inter*molecularly H-bonded aggregates as methanol dimers, trimers and high polymers [1,2], ethanol dimers [3] and water dimers [4], by carrying out ν_{OH} resonant irradiation coupled with FTIR spectroscopy and calculations. Over the past three years, we have also studied *intra*molecularly H-bonded molecules as acetylacetone [5] and malonaldehyde because they are the two most simple molecules which exhibit an *intra*molecular proton transfert. After deposition we observe only the chelated form in the matrix while after UV $\pi^* \leftarrow \pi$ resonant irradiation the *intra*molecular H-bond is broken leading to open-forms on which ν_{OH} resonant irradiation have been carried out provoking their interconversions. These UV and IR photoreactivities between all the isomers of each of these model molecules led us to suggest both their electronic and vibrational assignments.

The next step will be the recording of time-resolved IR spectra in a time range comprised between 70 ns and 100 ms in order to approach the reactional pathways involved in the vibrational or electronic relaxation phenomena.

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P2.33

EXPERIMENTAL AND COMPUTATIONAL STUDY OF BLUE-SHIFTING HYDROGEN BONDS: HXeY···HY COMPLEXES (Y = Cl and Br)

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Noble gas hydride molecules, with the general formula of HNgY (H = hydrogen atom, Ng = noble gas atom, and Y = electronegative fragment), have been a subject for experimental and theoretical studies since their discovery about ten years ago. This new group of molecules is found to have unusual properties, e.g. a very large dipole moment due to their strong ion-pair character.

HNgY molecules are very sensitive to the local surroundings and their complexes show large blue shifts of their H-Ng stretching vibrations. After studying several HNgY complexes ($HArF\cdots N_2$, $HXeCCH\cdots CO_2$, and $HXeOH\cdots H_2O$ etc.)[1-4], we concluded that the blue shift is a usual effect for this group of molecules. This interesting property of these molecules makes them benchmark systems to study physical reasons of blue-shifting hydrogen bonding.

In the present work, the complexes of HXeCl and HXeBr with HCl and HBr molecules have been studied. Computationally we found three complex configurations where HBr is connected to hydrogen or halogen end of HXeY (Y = Cl, Br) molecules. The studied molecules show exceptionally large values (> 100 cm^{-1}) of blue shifts in the H-Xe stretching frequency. The BSSE corrected interaction energies of different geometries varies from 100-2800 cm^{-1}. Matrix isolation experiments reveal formation of such blue-shifting complexes.

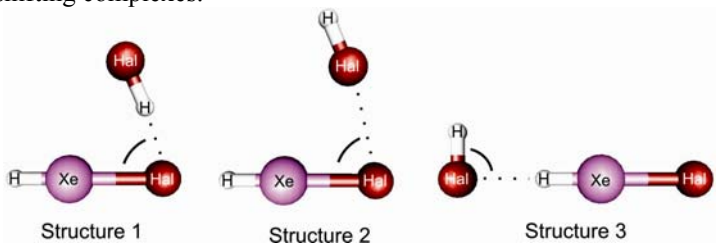

Figure 1. Computational minimum-energy structures of the HXeY···HY (Y = Cl and/or Br) complexes.

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P2.34

WEAKLY-BONDED COMPLEXES OF FORMIC ACID

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Formic acid dimer is the simplest organic system that can form two hydrogen bonds. As a model for large biochemical systems such as proteins it could be used to study of conformational structure and dynamics.As shown earlier, formic acid monomer (FA) can exist in two stable conformers with 0° and 180° HCOH dihedral angels (Figure 1). In the present work we report the first preparation of *trans-cis* dimers and *cis*-FA-water complex (FAW) in an Ar and Ne matrix. We show that the *trans-cis* dimers decay to the *trans-trans* form, but the decay rates differ from the reaction for the FA. The *cis-trans* dimers and *cis*-FAW are produced by light-induced rotation of the free OH bond of the corresponded *trans-trans* form. The *cis-trans* dimers convert in dark back to the *trans-trans* forms, which presumably occur via tunneling mechanism similarly to FA. Sets of fundamental absorption bands of the *trans-trans* and *cis-trans* dimers were identified in Ar and Ne matrices. The decay of *cis*-FA is enhanced at elevated temperatures in Ar. In sharp contrast, practically no increase of the decay rate was observed for the tc1 in this temperature range, and at 30 K it is ~30 times more stable than the *cis*-FA. As for tc4 it behaves like *cis*-FA at elevated temperatures but at low it is similar to tc1. The proton tunneling decay of *cis*-FA monomer is surprisingly very fast in solid neon, two orders of magnitude faster than in solid argon. It was found that the stability of the *tc1* against proton tunneling is enormously enhanced compared to the *cis*-FA by a factor of 300. Unless dimers, the *cis*-FAW doesn't tunnel back in daytime scale. These results show that hydrogen bonding can terminate tunneling reactions and efficiently stabilize intrinsically unstable conformational structures in complex asymmetrical hydrogen-bonded networks.

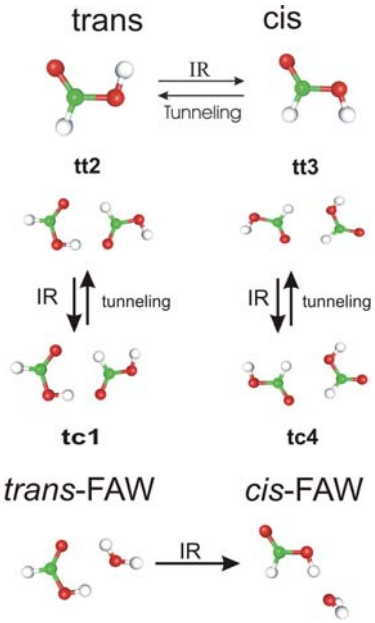

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Figure 1. Conformers of formic acid (HCOOH), formic acid dimers, trans-FAW and cis-F

P2.35

IINS, IR AND DFT INVESTIGATIONS OF VIBRATIONAL SPECTRA AND HYDROGEN BONDS IN 3,3-DIMETHYL-1-BUTANOL AND 3,3-DIMETHYL-2-BUTANOL

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The 3,3-dimethyl-1-butanol (3,3-DM-1B) and 3,3-dimethyl-2-butanol (3,3-DM-2B) are isomers of neohexanol of chemical formula $C_6H_{13}OH$. Both alcohols are glass forming substances. At low temperature in 3,3-DM-1B glass of isotropic liquid phase or crystal phase was detected depending on a cooling rate while for 3,3-DM-2B [1] only glass of plastic crystal was observed.

Inelastic incoherent neutron scattering (IINS) method gives mainly information about low frequency methyl motions and vibrational dynamics in the investigated compounds. Experimental phonon density of states $G_{exp}(\nu)$ in the frequency range up to 1600 cm^{-1} was obtained after transformation of the IINS spectra in one-phonon scattering approximation. The neutron spectroscopy studies have been completed by results of the far infrared spectroscopy (FIR) obtained in the frequency range 40-500 cm^{-1} (for 3,3-DM-2B only), and of the middle infrared spectroscopy (MID) in the frequency range 400-4000 cm^{-1} (for both substances). The temperature dependence of the $G_{exp}(\nu)$ and FIR absorption spectra was investigated in the temperature range of 20-300 K. The MID spectra of two investigated isomers have been measured in the liquid phase at the room temperature. In MID spectra for 3,3-DM-1B and 3,3-DM-2B the harmonic OH stretching mode ν_{OH} was detected at 3340 cm^{-1} and 3392 cm^{-1}, respectively. Therefore one may conclude that the hydrogen O-H…O bonds in 3,3-DM-1B are stronger than in 3,3-DM-2B as was expected due to the OH group position in the molecules. Taking into account correlations between O-H stretching modes and hydrogen bond length as proposed by Novak [2], the estimated hydrogen bond length for 3,3 DM-1B and 3,3 DM-2B are 2.76 Å and 2.80 Å, respectively.

The density functional theory (DFT) calculation methods were used for assignment of the vibrational bands observed in the $G_{exp}(\nu)$ and in the absorbance optical spectra. Geometry of isolated molecules, as well as of dimer and trimer molecular chains for both studied alcohols was optimised using the Gaussian03 program [3] on the B3LYP level with 6-311G** basis set [4,5]. The frequencies and intensities of the normal modes were calculated as well. The $G_{cal}(\nu)$ spectra calculated in isolated molecule approximation are in qualitative agreement with the experimental $G_{exp}(\nu)$. The frequency of bands corresponding to the hydrogen bond excitations have been predicted basing on vibrational spectra calculated for dimers and trimers of both studied alcohols. The frequencies of vibrations corresponding to the out-of-plane and the in-plane modes of the O-H…O bond were estimated in the range of (358-562) cm^{-1} and (954-1275) cm^{-1} for 3,3-DM-1B, and in range (280-630) cm^{-1} and (1027-1091) cm^{-1} for 3,3-DM-2B. The experimental FIR and MID spectra confirm the predicted frequency values.

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The calculations have been performed at the PCSC in Poznan.

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