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Fields of research

- Bioremediation of organic pollutants in soil and sewage
- Immobilization of biocatalysts, living cells or enzymes, into organic or organic-inorganic matrices by sol-gel process
- Application of immobilized biocatalysts in optical sensors
- Polymeric antidegradants immobilized on poly(siloxanes)
- Structure, reactivity, and catalytic properties of azine diphosphine complexes of transition metals
- Catalysts for fluorous biphasic media
- Carbosilane dendrimers
- NMR spectroscopy

Applied research

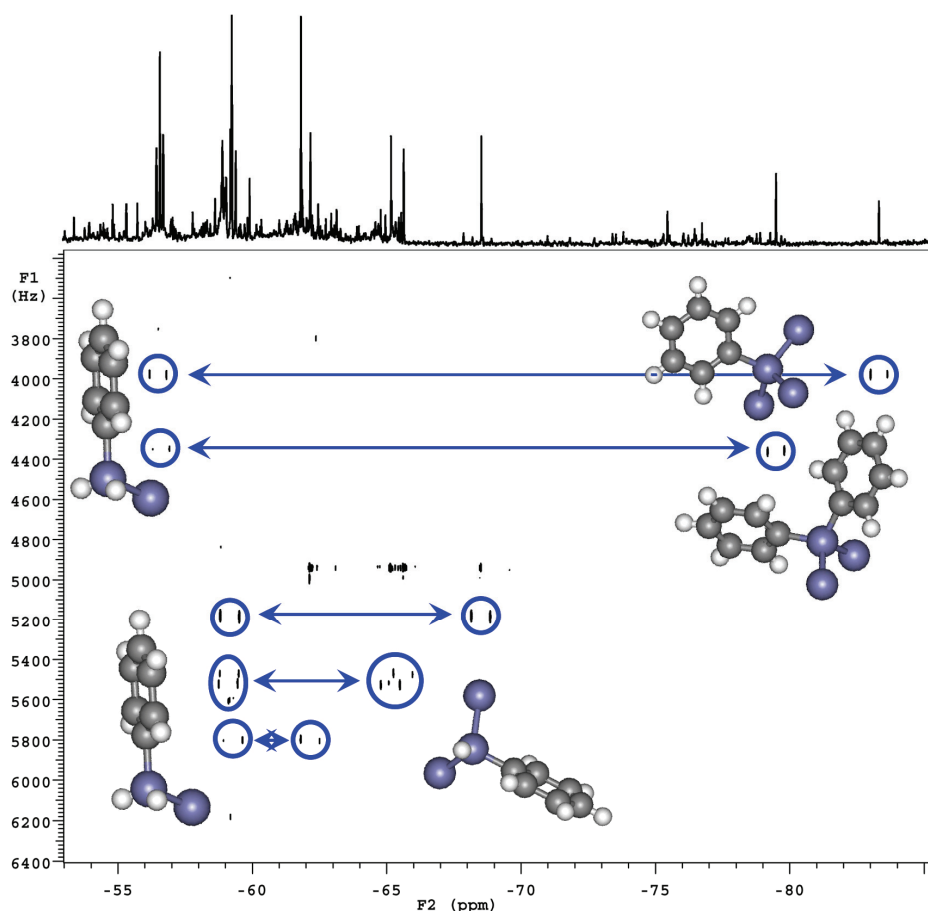
- Complex dehalogenation of PCB contaminated soils, waste water and oils
- Development of new analytical methods
- Analytical services to the research departments of ICPF

Research projects

Dehydrocoupling reactions catalyzed by titanium complexes

(J. Sýkora, joint project with JH IPC, and ICT, supported by GACR, grant No. GA203/09/1574)

Products of dehydrocoupling polymerization reactions were monitored by on-flow LC-NMR and GPC-NMR experiments. Several modifications of the $^{29}\text{Si}\{^1\text{H}\}$ INEPT experiment were implemented to probe the polymer microstructure. The 2D heteronuclear NMR experiments ($^1\text{H} \rightarrow ^{29}\text{Si}$ - ^{29}Si INEPT-INADEQUATE and $^1\text{H} \rightarrow ^{29}\text{Si}$ DOSY) provide valuable information about the branching and length of the oligosilanes. [Refs. 36, 48, 49]

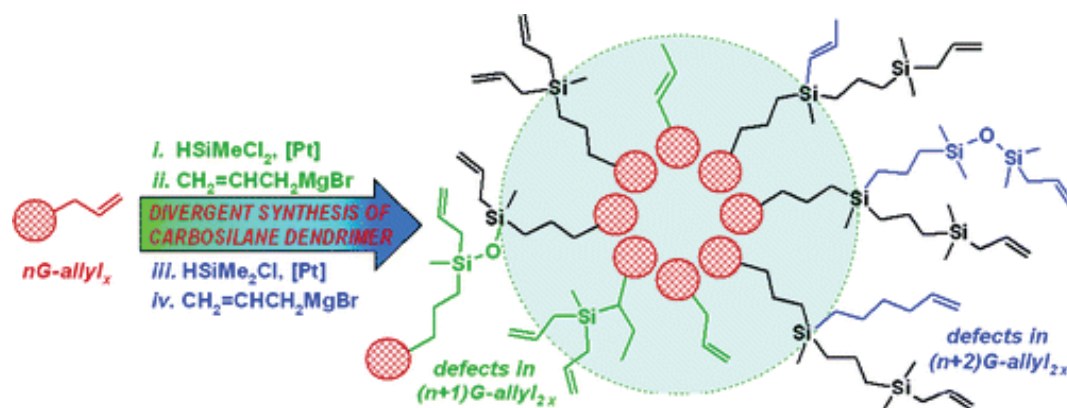


$^1\text{H} \rightarrow ^{29}\text{Si}$ - ^{29}Si INEPT-INADEQUATE experiment

The structure and synthetic applications of transition metal complexes

(J. Čermák, joint project with JH IPC, CU, and ICT, supported by MYES, project No. LC06070)

Two ways of immobilization of dichlorotitanocene units to carbosilane dendrimers were studied, the so called inverse and normal hydrosilylations. The normal hydrosilylation, i.e. hydrosilylation of an alkene terminated dendrimer with Si-H-bond-substituted complex gave better results provided that dendrimers were terminated by vinyl instead of allyl terminal groups. Complete analysis of defects in carbosilane dendrimers using combination of MALDI-TOF mass spectrometry and multinuclear NMR spectroscopy was also finished as a knowledge base for future design of dendrimeric structures. Coordination properties of heavy fluorine cyclopentadienes were studied as well. [Refs. 4, 5, 9, 21-25, 32, 47]

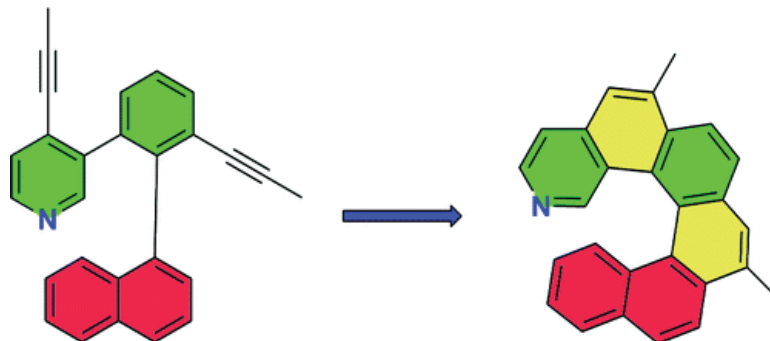


Structural defects in polyallylcarbosilane dendrimers

Synthesis of helicenes via cycloisomerization of biphenyl-naphthalene and 1,8-diarylnaphthalene derivatives

(J. Čermák, J. Storch, supported by GACR, grant No. P207/10/1124)

The new approach leading to 2-aza[6]helicene was developed being an extension of our previous work published in 2009. It focused on double cycloisomerization of biphenyl-naphthalene derivatives leading to formation of two aromatic rings in one step. During the last period we have found out a novel tandem cycloisomerization method giving rise to four new aromatic or heteroaromatic rings, yielding various benzo[c]phenanthrene and 6H-naphtho[2,1-c]chromene derivatives. This atom-economic isomerization is now being developed to the synthesis of extended [8]helicene-like molecules. [Refs. 15, 45, 46]

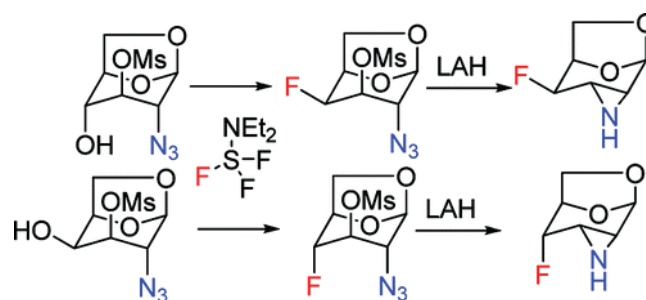


Synthesis of 2-aza[6]helicene utilizing metal-catalyzed cycloisomerization

Reactivity of asymmetrically substituted epimino pyranoses

(J. Karban, joint project with CU, supported by ICPF)

We have finished our work on aziridine-ring cleavage of 4-deoxy-2,3-epimino derivatives of 1,6-anhydro- β -D-hexopyranoses. The regioselectivity of the cleavage was found to be governed by interplay of $\text{S}_{\text{N}}2$ and $\text{S}_{\text{N}}2$ -borderline mechanism depending on the type of the nucleophile (hard versus soft) and conditions (acidic versus basic). To further investigate the cleavage mechanism we have prepared the full series of all configurational isomers of 4-fluoro-2,3-epimino-1,6-anhydro- β -D-hexopyranoses. These fluoro compounds were prepared by reaction of suitable azido sulfonates containing a free 4-hydroxyl with diethylaminosulfur trifluoride and subsequent reductive cyclization. The study of their reactivity is now in progress. [Refs. 7, 12, 13, 16, 30, 31, 37, 42, 43, 51]

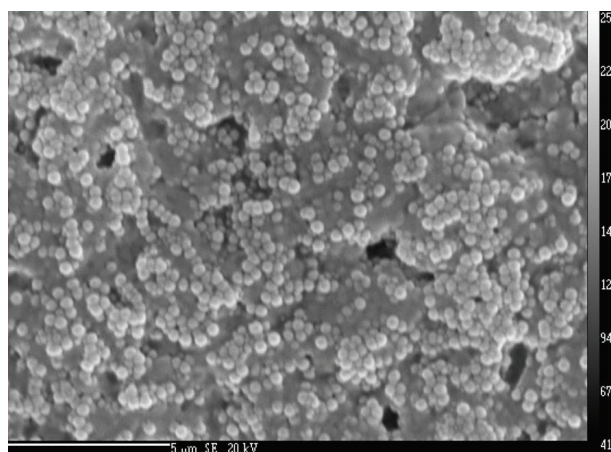


Synthesis of 1,6-anhydro-2,3,4-trideoxy-4-fluoro-2,3-epimino- β -D-hexopyranoses

Monitoring and remediation of environmental pollution with advanced organic-inorganic materials – MOREPIM

(G. Kuncová, supported by MEYS, KONTAKT project No. ME 892)

The research has been focused on utilization of inorganic and organic-inorganic nanoparticles in design of optical fibre sensors for monitoring of environmental pollution [Ref. 11, 17, 29, 34, 52].

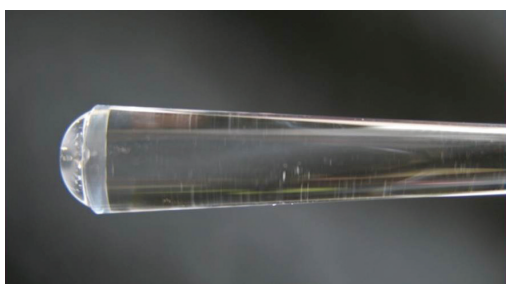


Fixation of bioluminescent bioreporters with silica nanoparticles

Whole cell optical sensors (WOCOS)

(G. Kuncová, supported by MEYS, KONTAKT project No. ME 893)

Bioluminescent bioreporters were immobilized on front faces of optical fibres with aim to prepare optical fibre sensors for in situ monitoring in remote localities. We calculated that only 3.5% of all photons, produced by one bacterium placed on the front end of the optical fibre are coupled and guided. Up to six times higher intensity of detected light was calculated and measured by enlargement of an area covered with bacteria using the front face of optical fibre with appropriate shape. [Refs. 2, 33, 40, 52]

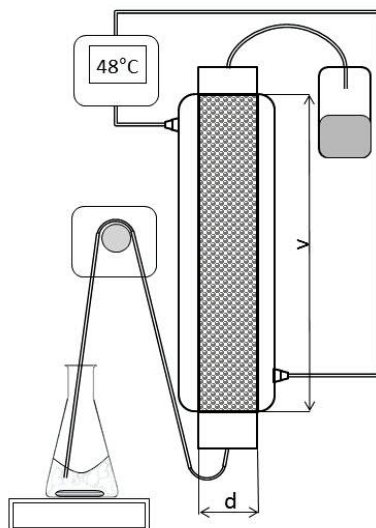


The tip of tapered quartz optical fibre ($\text{\O} = 10 \text{ mm}$) coated with *Pseudomonas putida* TVA8 encapsulated in silica gel

Enzymatically catalyzed synthesis of alkyd resins (ENZALKYD)

(G. Kuncová, joint project with SYNPO Pardubice a.s., supported by MIT, project No. MPO 2A-3TP1/108)

The research has been focused on continuous glycerolysis of soybean oil catalyzed with immobilized enzyme in column reactor. [Refs. 19, 20]

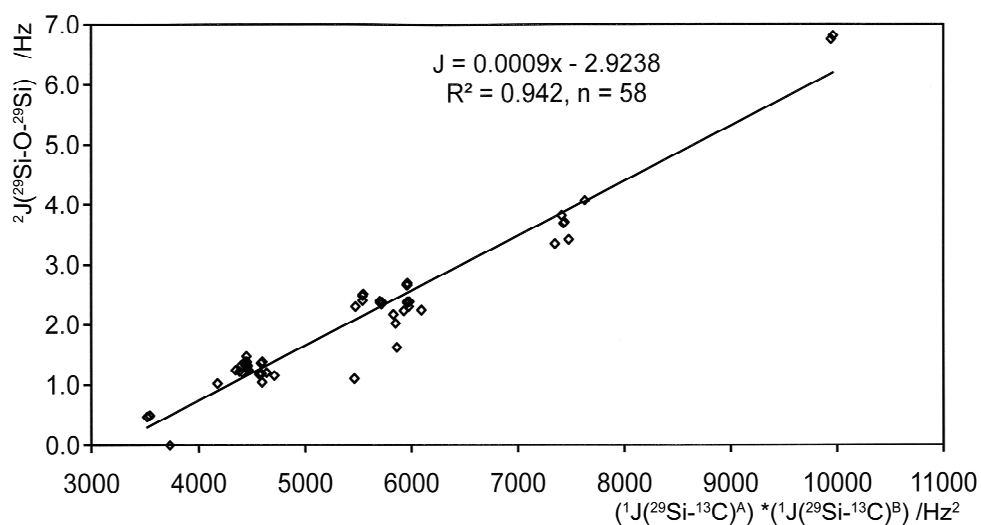


Column reactor for continuous glycerolysis of vegetable oils catalyzed with immobilized lipase

²⁹Si-NMR structural analysis of branched organosilicon polymers and its application in LC-NMR

(J. Kurfürst, supported by GACR, grant No. GP203/08/P412)

²⁹Si-O-²⁹Si coupling constants were determined for a series of 56 siloxanes and empirical correlations were found between these couplings and number of oxygen atoms attached or the sum of ²⁹Si chemical shift. The correlation with the product of ¹J(²⁹Si-¹³C) couplings was put on a theoretical basis. [Ref. 3]

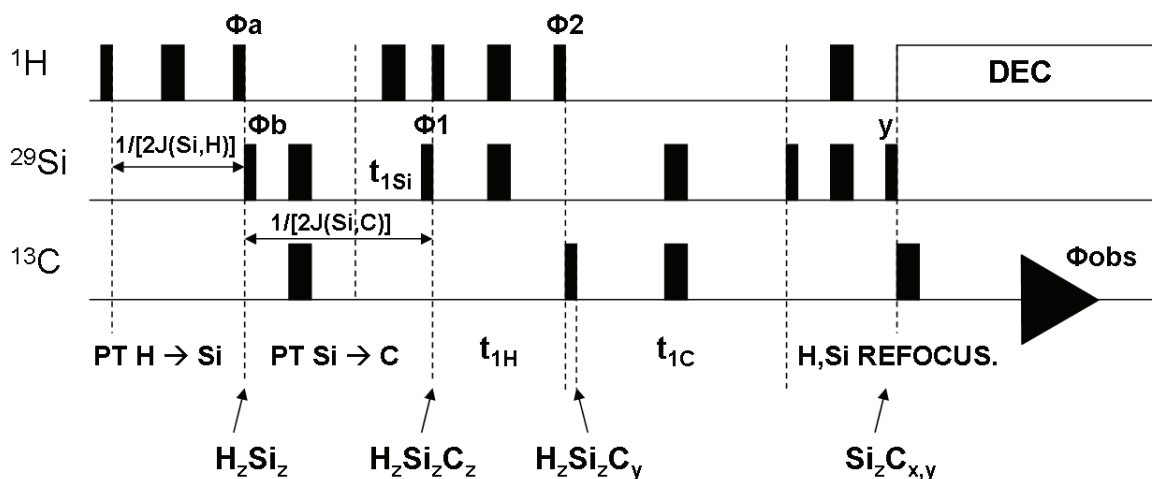


Correlation between geminal two-bond coupling $^2J(^{29}\text{Si}-\text{O}-^{29}\text{Si})$ and one-bond couplings $^1J(^{29}\text{Si}-^{13}\text{C})$ in methylsiloxanes

Structure of silyl moieties through $J(^{29}\text{Si}-^{13}\text{C})$ couplings as determined by triple $\{^1\text{H}, ^{13}\text{C}\}^{29}\text{Si}$ NMR experiment

(J. Schraml, supported by ASCR, grant No. IAA400720706)

New methods for measurement of signs of spin-spin couplings between ^{29}Si and ^{13}C or ^1H nuclei in solutions utilize instrumental possibilities of triple resonance of ^1H - ^{13}C - ^{29}Si nuclei. Using these experiments model series of compounds have been measured [Refs. 1, 10, 18, 44].

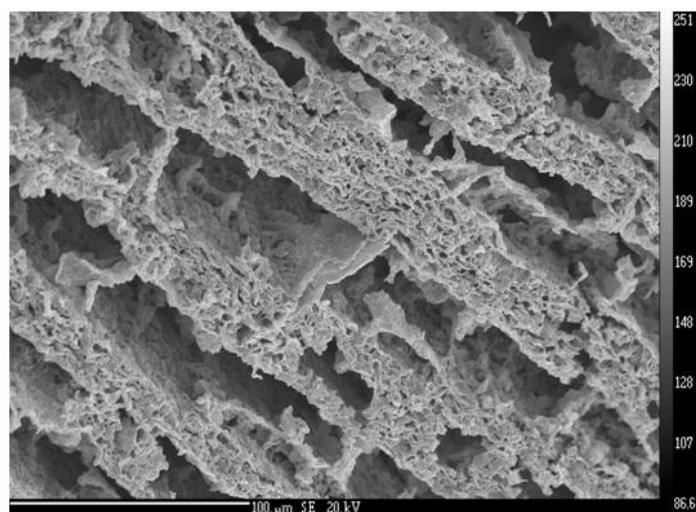


NMR Pulse sequence for determination of the signs of heteronuclear coupling constants

Novel inorganic-organic hybrid nanomaterials

(S. Šabata, joint project with ICT Prague, IMC, University of West Bohemia Plzeň, supported by ASCR, grant No. IAAX08240901)

Na^+ montmorillonite was silanized with methoxy- and ethoxy- organosilanes having functional groups; $-\text{C}_3\text{H}_7\text{NH}_2$, $-\text{CH}_2\text{CH}=\text{CH}_2$, $-\text{C}_8\text{H}_{17}$, $-\text{C}_{18}\text{H}_{37}$, $-\text{C}_3\text{H}_7\text{C}\equiv\text{N}$. The products were characterized with X-Ray. Enzyme lipase was adsorbed on modified montmorillonites. The highest catalytic activity, in esterification of stearic acid with propanol, performed biocatalyst prepared by adsorption of Lipolase 100L on montmorillonite with $-\text{C}_{18}\text{H}_{37}$. [Ref. 6, 8, 26-28, 33, 50]

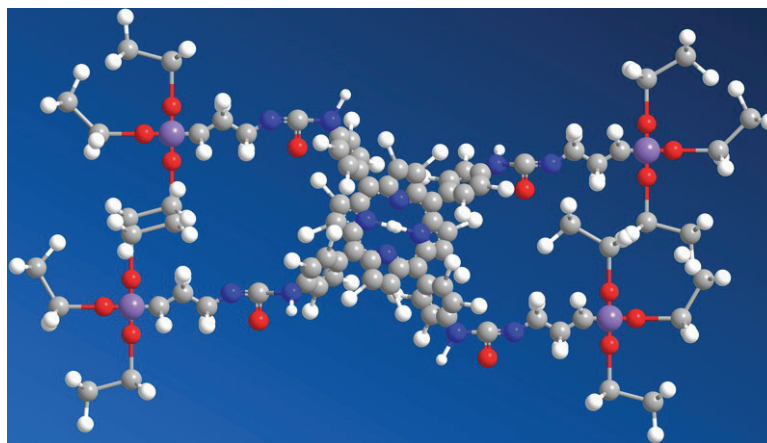


The SEM micrographs of cross sections of lipase catalyst (cloisite modified with octadecyltrimethoxysilane) formed by ice-templating processes

Calixarene-porphyrin conjugates for selective complexation and separation of fullerenes

(S. Šabata, joint project with ICT, IIC, supported by GACR, grant No. 203/09/0691)

Novel technique of silanization of aminoporphyrines and thiacalixarenes was developed. The silanization products of tetraaminoporphyrine and thiacalixarene were characterized with $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ spectroscopy. Silanized tetraaminoporphyrine was immobilized on silica carrier and this material has been tested as filling of HPLC column. [Ref. 50]



Silanized tetraaminoporphyrine

International co-operations

Centre for Environmental Biotechnology, University of Tennessee, Knoxville, TN, USA:

Improved biomaterials for the encapsulation of living cells

Environmental Sciences Division Oak Ridge National Laboratories, Oak Ridge, TN, USA:

Application of nanomaterials and novel organic-inorganic materials in optical sensors

Graz University of Technology, Graz, Austria: ^{29}Si and ^{119}Sn NMR

Instituto Superior Técnico, Lisbon, Portugal: Chemistry of transition metal complexes with azine ligands

Teaching

J. Čermák: UJEP, Faculty of Science, courses “Organic chemistry I and II”, “Chemistry of heterocyclic and organometallic compounds”, “Introduction to the spectral methods in organic chemistry”

G. Kuncová: ICT, Faculty of Chemical Engineering, postgraduate course “Optical sensors for measurement in chemical and biological reactors”

Publications

Original papers

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Chapters in books

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International conferences

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