

Technical Report

Calix 2007: 9th International Conference on Calixarene Chemistry

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The DOE funds helped support an International Conference, **Calix 2007**, whose focus was on Supramolecular Chemistry. The conference was held at the University of Maryland from August 6-9, 2007 (**Figure 1**). The conference website is at www.chem.umd.edu/Conferences/Calix2007. This biannual conference had previously been held in the Czech Republic (2005), Canada (2003), Netherlands (2001), Australia (1999), Italy (1997), USA (Fort Worth, 1995) Japan (1993) and Germany (1991). Calixarenes are cup-shaped compounds that are a major part of Supramolecular Chemistry, for which Cram, Lehn and Pederson were awarded a Nobel Prize 20 years ago. Calixarene chemistry has expanded greatly in the last 2 decades, as these compounds are used in synthetic and mechanistic chemistry, separations science, materials science, nanoscience and biological chemistry. The organizing committee was quite happy that **Calix 2007** encompassed the broad scope and interdisciplinary nature of the field. Our goal was to bring together leading scientists interested in calixarenes, molecular recognition, nanoscience and supramolecular chemistry. We believe that new research directions and collaborations resulted from an exchange of ideas between conferees. This grant from the DOE was crucial toward achieving that goal, as the funds helped cover some of the registration and accommodations costs for the speakers.

Strengths of the Conference: The strengths of the **Calix 2007** conference included: a) the broad scope of the basic and applied research presented (e.g. electrochemistry, molecular machines, materials, nanoscience, biomimetics, drug delivery and many other areas) b) the stature of the many world-leading chemists that spoke, including Jerry Atwood, David Reinhoudt, Fraser Stoddart, Makoto Fujita, Luis Echegoyen and Kimoon Kim, among others; c) the international diversity of the speakers, including scientists from the USA, South Korea, Japan, China, France, Spain, Germany, Italy, Netherlands, Czech Republic, England and Israel; d) the significant number of younger speakers, including Michael Hardie, Galina Talinova, Christophe Schalley, Ralf Warmuth, Travis Holman and Takeharo Haino, among others; e) the richness of the poster sessions which were displayed in the Conference Center's main concourse during the entire 4-day period, enabling much interaction.

The **Calix 2007** conference, where a diverse group of researchers shared ideas and form new collaborations, enhanced the development of relationships between US and international scientists. This meeting also benefitted the development of younger scientists, as they had the opportunity to interact with many of the experts who developed the field. The conference featured 6 half-day sessions, each with its own focus.

Below, are the conference themes and speakers:

A) Molecular Containers, Capsules, Cages and Catenanes

Jerry Atwood, University of Missouri, **USA**

"Supramolecular Encapsulation of Gases"

Javier de Mendoza, Institute of Chemical Research of Catalonia, **Spain**

"Trapping Cavitands Inside of Calixarenes"

Makoto Fujita, University of Tokyo, **Japan**

"Cages from Metal Atoms"

Yiu Liu, Nankai University, **China**

“Assemblies of Sulfonatocalixarenes: Capsules versus Bilayers”

Volker Bohmer, University of Mainz, **Germany**

“Rotaxanes and Catenanes from Self-Assembling Calixarenes”

B) Physical Organic Chemistry inside Capsules

Ralf Warmuth, Rutgers University, **USA**

“Solvent and Isotope Effects Inside Nanocontainers”

Travis Holman, Georgetown University, **USA**

“Selective Anion Encapsulation by a Cryptophane with a Pi-Acidic Interior”

Bruce Gibb, University of New Orleans, **USA**,

“Water Soluble Nanocapsules that Bind Hydrocarbons”

Takeharu Haino, Hiroshima University, **Japan**

“A New Calix[5]arene-Based Container: Selective Extraction of Higher Fullerenes”

Angel Kaifer, University of Miami, **USA**

“Molecular Shuttles: pH-Controlled Pseudorotaxanes based on Cucurbit[7]uril”

C) Ion Recognition and Separation

Pavel Lhotak, University of Prague, **Czech Republic**

“Structure, Dynamics and Applications of Thiocalixarenes”

Jonathan Sessler, University of Texas, **USA**

“Calixpyrroles-Anion Recognition and Transport”

Bruce Moyer, DOE Oak Ridge National Labs, **USA**

“Anion Coordination in Metal-Organic Frameworks”

Phil Gale, University of Southampton, **England**

“Molecular Recognition with Acyclic Anion Receptors”

D) Supramolecular Analysis

Christophe Schalley, University of Bonn, **Germany**

“Supramolecular Chemistry in the Gas Phase”

Iris Thondorf, University of Halle, **Germany**

“Molecular Dynamics on Molecular Containers”

Yoram Cohen, University of Tel Aviv, **Israel**

“NMR of Molecules at Close Range: Encapsulated Solvent Molecules in Capsules”

Michaele Hardie, University of Leeds, **England**

“Synthesis and X-Ray Structural Studies of Cyclotrimeratrylenes”

Galina Talinova, Howard University, **USA**

“Rigid versus Flexible? Conformation and Recognition by Calix[4]arenes”

E) Nanoscience from the “Bottom-Up” and the “Top Down”

David Reinhoudt, University of Twente, **Netherlands**

“Molecular Printboards”

Fraser Stoddart, UCLA, **USA**

“Molecular Solomon Links”

Enrico Dalcanele, University of Parma, **Italy**

“Grafting Cavitands onto Surfaces”

Luis Echegoyen, Clemson University, **USA**

“ Nanoassembly of Fractal Polymers ”

Dmitry Rudkevich, University of Texas-Arlington, **USA**

“ Supramolecular Polymers from Calixarenes ”

F) Biological Applications of Calixarenes and Related Molecules

Thomas Schrader, University of Duisberg-Essen, **Germany**

“DNA Recognition by Calixarenes ”

Alessandro Casnati, University of Parma, **Italy**

“DNA Condensation and Cell Transfection Properties of Guanidinium Calixarenes ”

Kimoon Kim, Pohang University, **South Korea**

“Functionalized Cucbiturils and their Applications ”

Olivia Reinaud, Rene Descartes University, **France**

“Supramolecular Systems For Modeling Metalloprotein Active Sites ”

In addition to invited speakers, 4-5 younger researchers were asked to present 10-minute talks during a special session. These short talks were chosen based on the quality of the submitted posters.