Dr. Cornelia Bohne, ***Professor***

(é brasileira, formada pela USP mas é professora no Canadá desde 1992))

Pesquisa abrange temas relacionados com química, física, biologia.Participa ou participou recentemente do órgão equivalente ao CNPq no Canadá

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Cornelia Bohne was born in São Paulo, Brazil, and studied chemistry at the Instituto de Química of the Universidade de São Paulo. She pursued her graduate studies at the same University under the supervision of Professor Giuseppe Cilento, where she studied the mechanism for the enzymatic generation of triplet excited states and the energy transfer from excited states to acceptors bound to biomolecules. She obtained her Ph.D. in 1987. As a post-doctoral fellow Dr. Bohne worked with Professor Tito Scaiano at the National Research Council of Canada and the University of Ottawa. During this period she studied the photochemistry of compounds in homogenous solution and in microheterogeous systems, such as reversed micelles, cyclodextrins and cells.

In 1992 Dr. Bohne accepted a position as Assistant Professor at the Department of Chemistry, University of Victoria. She obtained tenure and was promoted to Associate Professor in 1997 and to Full Professor in 2000. In 1998/99 Dr. Bohne was an

Alexander von Humboldt Research Fellow at the Fritz-Haber Institut der Max-Planck Gesellschaft in Berlin, working with Professor Josef Holzwarth.

Dr. Bohne's research interests are in supramolecular dynamics. Supramolecular architectures are organized by intermolecular forces between components, and can achieve functions that are not possible for the individual building blocks. In contrast to molecular chemistry, supramolecular systems are always reversible, and dynamics are essential to achieve function. Dr. Bohne's long-term goal is to bring the understanding of supramolecular dynamics to the same level as its structural aspects. Knowledge of the underlying concepts for supramolecular dynamics is vital to fulfill the longstanding promise that these systems can lead to functions inaccessible to molecular chemistry. In her studies Dr. Bohne measures events in real-time, using fast kinetic techniques, including laser flash photolysis, stopped-flow and laser temperature-jump experiments. For each supramolecular system her group develops the required methodology to measure dynamics in real-time, establishes the relationship between dynamics and structure of the supramolecular building blocks, and applies this knowledge to design new supramolecular functions. The supramolecular systems currently under investigation are cyclodextrins, bile salt aggregates, DNA and proteins.

Dr. Bohne has served in several peer review capacities. From 1999 to 2002 she was a member of the Inorganic-Organic Grant selection committee (one of the two national committees in chemistry) at the Natural Sciences and Engineering Research Council of Canada, and she chaired the committee for the 2001-2002 grant competition. She is currently Associate Editor of Photochemistry and Photobiology and is on the Editorial Advisory Board of Langmuir. At the administrative level, Dr. Bohne has recently served as the acting chair of the Chemistry Department from July to December 2002.

Other scholarly activities include Dr. Bohne's involvement in the Inter-American Photochemistry Society as a former member of the advisory board, current Canadian treasurer, member of the several organizing committees for IAPS conferences, and as co-chair of the IAPS conference in 2004. She is also involved in IUPAC as a member of the Canadian National Committee for IUPAC and as a member of the IUPAC Sub-Committee on Photochemistry. Dr. Bohne is a founding member of the Reactive Intermediate Student Exchange program.

RESEARCH in SUPRAMOLECULAR DYNAMICS

Supramolecular chemistry is an exciting and developing field where new functions are explored. Supramolecular architectures are organized by intermolecular forces between components. These structures can achieve functions that are not possible for the individual building blocks. An analogy to the macroscopic world is that bricks, doors and windows by themselves are of limited use, but when organized into a house can provide shelter.

In contrast to molecular chemistry, supramolecular systems are always reversible, and dynamics is essential to achieve function. A large number of supramolecular architectures have been synthesized and their structural complexity continues to rapidly increase. Most of these systems have been characterized using static techniques, such

as structural and thermodynamic studies. In the analogy drawn with houses, these static techniques provide a great number of photographs of buildings with different shapes, but nothing can be known on how fast doors and windows open and how fast people enter these buildings and can move within them.

Our long-term goal is to bring the understanding of supramolecular dynamics to the same level of understanding as its structural aspects. Knowledge of the underlying concepts for supramolecular dynamics is vital to fulfil the longstanding promise that these systems can lead to functions inaccessible to molecular chemistry. Our studies will provide the video which detail the action and not only snapshots of the shapes.

In supramolecular dynamics we measure events in real-time, using fast kinetic techniques, including laser flash photolysis, stopped-flow and laser temperature jump experiments. For each supramolecular system we develop the required methodology to measure dynamics in real-time, establish the relationship between dynamics and structure of the supramolecular building blocks, and apply this knowledge to design new supramolecular functions.

Cyclodextrins (CDs) are very popular host molecules in supramolecular chemistry because of their defined shape and ready availability. The thermodynamics of complexation are well established. Our studies on the dynamics of 1:1 (guest:CDs) complexes established that the association and dissociation processes are faster than tenths of microseconds and are influenced by the size complementarity between guest and host, chemical nature or shape of the guest, and modifications to the CD structure. The dynamics of complexation for structures containing more than one CD is surprisingly slower, frequently occurring in the millisecond to second time domain. This feature is currently being explored to improve chiral recognition and to achieve the kinetic control of self-assemblies.

Bile salt molecules are amphiphilic and they form complex aggregates in water. Our studies on the dynamics of guest binding to bile salt aggregates showed that bile salt aggregates have defined binding sites with different properties. This is a landmark observation clearly establishing that bile salt aggregates are not micelles and possess superior properties that can be exploited for supramolecular function. We are currently performing structure-dynamics studies to establish how the binding dynamics are affected by the topology, hydrophobicity and hydrogen bonding ability of the guest and the structure of the bile salts.

Dynamics of guests with DNA and proteins is being investigated. These projects are at the stage where methodology is being developed. The long-term objective is to establish if there is a relationship between dynamics and biological function.

Projetos:

A range of projects is available from the development of kinetic techniques, physical-organic mechanistic studies, and projects involving some synthesis.

Cyclodextrins:

- Studies on structural requirements to enhance chiral recognition.
- Kinetic control of self-assembly of complexes containing more than one cyclodextrin.
- Studies on the slow complexation dynamics using laser temperature jump (see below).

Bile salt aggregates:

- Structure-dynamics relationship studies.
- Use of bile salt aggregates to manipulate chemical reactivity.
- Chiral recognition.

DNA:

- Dynamics of guest intercalation into DNA.
- Structure-dynamics relationship studies.

Proteins:

- Development of two-laser experiments to study the mobility of small molecules through protein matrixes.
- Mobility of guests using laser temperature jump experiments.

Joint-project with R.H. Mitchell:

Mechanistic studies on the photochromism of dimethyldihydropyenes (synthesis is done in the Mitchell group while the photochemistry/photophysics is studied in the Bohne group).

Development of the laser temperature jump technique:

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