



9th CANADIAN SYMPOSIUM ON THEORETICAL CHEMISTRY
e SYMPOSIUM CANADIEN SUR LA CHIMIE THEORIQUE

INTERNATIONAL CONFERENCE INTERNATIONALE

1986 June 23 - 27 juin

Toronto, Ont.

GENERAL CONFERENCE INFORMATION

The 9th Canadian Symposium on Theoretical Chemistry will be held on June 23-27th, 1986, at Trinity College, University of Toronto.

CONTRIBUTED PAPERS

Contributed papers will be welcome from all areas of theoretical chemistry. All contributed papers will be presented in poster format. Abstracts should be typed on the enclosed sheet in accordance with the instructions given there.

REGISTRATION

The registration fee includes full participation in the conference, the book of abstracts, complementary coffee breaks, and the conference banquet on Thursday evening.

The registration desk will be open from 2:00 p.m. to 6:30 p.m. on Sunday June 22nd, in the front hall of St. Hilda's residence (see enclosed campus map). On Monday, June 23rd, and for the remainder of the week, the registration desk will be open from 8:30 a.m. to 4:00 p.m. just outside the lecture hall (George Ignatieff Theatre).

ACCOMMODATION

University residence, St. Hilda's, Trinity College

If you have requested University accommodation you should go directly to the St. Hilda's College residence, 44 Devonshire Place and go to the Porter's desk at the front entrance. He will then give you the key to your room. A \$5.00 deposit is required, which will be refunded when you return the key at the end of the conference.

Park Plaza

The Park Plaza Hotel is situated at 4 Avenue Road (north west corner of Bloor and Avenue Road). Register in the normal way. Room rate is \$78.00 single/double.

Co-Chairmen/Co-présidents:

R. Kapral
Department of Chemistry
University of Toronto
Toronto, Ontario, Canada
M5S 1A1
Tel. (416) 978-6106

or

J. Paldus
Department of Applied Mathematics
University of Waterloo
Waterloo, Ontario, Canada
N2L 3G1
Tel. (519) 888-4412

TRAVEL

By Air

Toronto is served by most major airlines and is easy to reach by direct flights from Europe and the United States.

Transportation from the airport is readily available. Airport buses provide a regular direct service to the downtown area. The best bus is the Gray Coach from the Departure level to Yorkdale Station, then take the subway south to Museum, which is close to both the Park Plaza and Trinity College (see map). Cost \$4.00. There are always limousines waiting at the Departure level. The cost to the downtown area is approximately \$24.00.

By Train

If you are travelling by train to Union Station, it is a short subway ride from there to Museum Station. A single subway fare is \$1.00 but it is best to purchase token, 5 for \$4.00.

The University of Toronto is located in the heart of the city and is accessible by subway and surface transportation from most parts of the city.

By Car

Travellers who will be driving to Toronto require a driver's licence from any country, which is valid for 3 months. If driving a borrowed car, bring a letter from the owner, and if you are driving a rented car, a copy of the rental contract. Parking is available at the University in the St. George Street parking lot behind St. Hilda's College at the rate of \$4.00 per day.

CUSTOMS REGULATIONS

For customs regulations as they apply to visitors entering Canada please consult the nearest Consulate or Embassy of Canada, or write to: Customs and Excise Branch, Revenue Canada, Connaught Building, Mackenzie Avenue, Ottawa, Ontario K1A 0L5.

INSURANCE

Visitors are strongly advised to check that they have complied with all requirements both for entry into Canada and for their return journey.

Visitors are not covered by Canadian Health Insurance Plans. It is therefore recommended that participants arrange their own personal health and accident insurance. This can generally be done in the home country but those wishing to do so may obtain information and application forms for visitor's insurance from Ontario Blue Cross, 150 Ferrand Drive, Don Mills, Ontario M3C 1H6 or by telephone at (416) 429-2661. The rate is \$3.00 for single coverage per day and \$6.00 for family coverage per day.

General

No responsibility can be assumed for personal accidents, sickness, theft or property damage on behalf of delegates. Delegates are advised to take out insurance as they consider necessary.

PASSPORTS AND VISAS

Participants are strongly advised to determine their individual requirements with respect to entering Canada. Citizens of some countries require non-immigrant visas in addition to passports. Persons from outside the U.S.A. wishing to enter the U.S.A. from Canada should make arrangements before leaving their home country. Multiple entry visas are required if entering Canada and/or the U.S.A. more than once. U.S. citizens do not require passports or visas to enter Canada, but may be asked to prove their citizenship; a birth certificate or voter's registration card is adequate. Registered aliens residing in the United States must have their Alien Registration Cards.

SOCIAL PROGRAMME

There will be a Wine and Cheese Reception on Sunday, June 22nd from 6:30 p.m. to 8:30 p.m. in Seeley Hall, Trinity College, with a cash bar (2 free drinks will be provided by the Symposium).

There will be a free afternoon on Wednesday, June 25th and following tours have been arranged:

- an afternoon excursion to McMichael Art Gallery in Kleinburg, Ontario
- an afternoon excursion to Niagara Falls and Niagara on the Lake
- an evening boat excursion on Lake Ontario with dinner at Captain John's (a boat restaurant moored in Toronto Harbour)

Please indicate on the attached form if you will be attending any of these excursions.

The Symposium Banquet will be held in Strachan Hall, Trinity College at 7:30 p.m. on Thursday, June 26th and will be preceded by a reception (cash bar) in Seeley Hall at 6:30 p.m. After the banquet there will be a slide show presented by the famous Canadian photographer, Mr. Budd Watson entitled "The Seasons - Georgian Bay".

INFORMATION ON LOCAL CUISINE

Toronto abounds with many excellent restaurants of every kind and description and there is a great selection surrounding University campus, especially for lunches. Dundas Street and Spadina Avenue are in China Town and within easy walking distance of Trinity College if you feel like Chinese food. Bloor Street, Yorkville Avenue and Cumberland Avenue have endless cafes and restaurants and there are also cafeterias on campus if you do not feel like walking. Mrs. McClelland will have a full list of all the restaurants within the area.

SCIENTIFIC PROGRAMME

Invited lectures will be given each morning and afternoon. A detailed scientific programme will be sent to you at a later date. A list of the invited speakers and the titles of their talks is given below:

INVITED SPEAKERS	SUBJECT
R.J. Bartlett	"Analytical Derivative Techniques in Coupled Cluster Approach"
C.W. Bauschlicher	"The Importance of Electron Correlation on Transition Metal Bonding"
E.R. Davidson	"Comparison of Experimental and Theoretical Determinations of Electron Density"
G.W.F. Drake	"Relativistic and OED Effects in Two-Electron Atom and Ions - Comparison of Theory and Experiment"
K.F. Freed	"Renormalization Group Theory of Polymers"
H. Fukutome	"Characterization of Localized Broken Symmetry Solutions, Solitons, Polarons and Breathers in the Time Dependent HF Equation of a One-Dimensional System and their Significance in the Lattice Dynamics and Electron Correlation in Polyenes and Polyacetylene"
L. Glass	"Bifurcation and Chaos in the Hearts of Chickens and Men"
E.J. Heller	"Spectroscopy with Photons and Particles: Correlation Functions and Semiclassical Nonlinear Dynamics"
J.T. Hynes	"Along the Reaction Coordinate in Solution"
J. Koutecky	"General Rules on the Structure of Small sp Metal Clusters"
R.D. Levine	"Algebraic Methods for Molecular Structure and Dynamics"
J. Oddershede	"The Polarization Propagator Method and Its Applications"
G. Patey	"Recent Advances in the Integral Equation Theory of Liquids and Solutions"
I. Procaccia	"Infinity of Scenarios for the Onset of Chaos in Lorenz-like Flows"

- J. Ross "Experiments and Theory on Chemical Instabilities"
- P.J. Rossky "Quantum Simulation of Aqueous Systems"
- D.R. Salahub "Metal Clusters Interacting with Adsorbates - The Local (Spin) Density Description"
- M. Shapiro "Coherent Control of Chemical Reactions"
- H.J. Silverstone "Beneath the Surface of Quantum-Mechanical Perturbation Theory: Divergence, Borel-Based Summability, Exponentially Small Subseries, and the Quasi-Semiclassical Method, with Theoretical and Practical Application to the LoSurdò-Stark Effect, the Hydrogen Molecule-Ion, and the JWKB Method"
- H. Swinney "Chemical Chaos and Intermittency"
- A.J. Thakkar "Quantum Chemistry in Momentum Space: An Overview"
- D.R. Truax "Supersymmetry"
- J.P. Valleau "Monte Carlo Study of a Model of a Flexible Polyelectrolyte"
- A. van der Avoird "A Quantum Chemical Approach to the Properties of Molecular Crystals"
- P. Wolynes "Beyond the Golden Rule: From Proteins in Semiconductors"
- M.C. Zerner "Characterizing Potential Energy Surfaces: Art and Science"

Contributed papers, from all areas of theoretical chemistry are welcome. The poster sessions will be scheduled in the afternoon. The attached abstract form should be consulted for additional information.