



Septième
Symposium
Canadien
sur la
Chimie
Théorique

Seventh
Canadian
Symposium
on
Theoretical
Chemistry

Co-chairmen / Co-présidents

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SEVENTH CANADIAN SYMPOSIUM ON THEORETICAL CHEMISTRY

BANFF CENTRE, BANFF, ALBERTA, CANADA

JUNE 15-20 1980

GENERAL

The response to the previous announcement has been encouraging. Between 150 and 200 scientists from many different countries have indicated their intention to attend the symposium. Additional requests for participation will be considered subject to the availability of accommodation; space for 60 minute poster sessions can still be arranged. Registration is now \$200 (regular) and \$150 (for graduate students and postdoctoral fellows). Interested individuals should phone the conference office [Mrs. Kokoski (403) 284-5051] or one of the chairmen without delay.

TRANSPORTATION

There will be a symposium information desk at the Calgary International Airport on Sunday, June 15 from 10:00 am to 10:00 pm. Banff Centre is located in Banff, 128 km west of Calgary. Transportation from the airport to Banff Centre will be provided by bus at a cost of \$8.00 per person. If symposium buses are not available at your arrival time, Brewster Gray Line runs a regular bus service between the Calgary International Airport and Banff (with drop off at the Banff Centre) at a cost of \$12.00. Banff is accessible by scheduled Greyhound Bus Lines and Via Rail Canada. Car rentals are available at the airport but it is suggested that you book ahead.

REGISTRATION

The registration fee includes full participation in the symposium, the reception on Sunday, June 15, and the Barbeque on Thursday, June 19.

Registration will take place on Sunday, June 15, from 15:00 to 22:00 in the Donald Cameron Hall of the Banff Centre, Banff, Alberta.

ACCOMMODATION AND FOOD

Accommodation is available at the Banff Centre at a rate of \$40.00 single and \$32.00 twin including 3 meals daily for all those who have sent in their accommodation forms to the Banff Centre. Meals are available at the Banff Centre for those who have booked accommodation elsewhere but the necessary tickets must be purchased at the Banff Centre.

PARKING

Free parking is available at the Banff Centre.

MIXER/RECEPTION

A reception will be held from 19:00 to 24:00 on Sunday evening, June 15, in the Donald Cameron Hall of the Banff Centre. A complimentary bar will be open from 19:00 to 22:00 at the reception.

BANQUET

On Thursday, June 19, a western style barbeque will be held at a Guest Ranch near Banff. Casual dress is suggested and participants are reminded that temperatures may drop to near freezing at night with daily highs of 20-25°C.

BUSINESS MEETING

There will be a business meeting of the Canadian Theoretical Chemists on June 19.

SCIENTIFIC PROGRAM

All sessions will be held in the Max Bell Building beginning at 8:30 am, June 16 through 20. Blackboard space, a 35 mm slide project, a 16 mm film projector and an overhead projector are available. A projectionist will be in attendance. Poster presentations should be prepared for presentation on a 4' x 8' display board.

The schedule for the invited talks is given in Table I and the titles of invited talks are provided in Table II. The schedule for shorter communications and the poster sessions will be available at the opening of the symposium. A listing of the authors, titles and abstracts of all presentations will be available at the registration desk on June 15.

ACTIVITIES

There are bus tours to Lake Louise and surrounding areas. Wednesday afternoon and evening have been kept free for excursions (e.g. Columbia Ice Fields). Since there are many hiking trails and nature trails in the vicinity you may wish to bring the appropriate gear (e.g. shoes, etc.). Shopping facilities and many other attractions are within walking distance of the Banff Centre. Additional information will be available at the Registration Desk but for advance planning one should write to the Banff Chamber of Commerce, 94 Banff Avenue, Banff, Alberta T0L 0C0, Canada.

Table I: Schedule of invited speakers and sessions for contributed papers.

Session/Section	June 16	June 17	June 18	June 19	June 20
Chairmen 8:30 - 9:15	F. Birss Opening <u>R. Kapral</u> H. Umezawa	<u>R. Snider</u> O.C. Rossler B. Clarke	<u>A. Hunding</u> P. Orteleva J. Turner	<u>R. Truax</u> C.E. Wulfman J. Paldus	<u>R. Paul</u> G. Mazenko P.R. Bunker
9:15 - 10:00	R. Desai	B. Clarke	J. Turner	J. Paldus	P.R. Bunker
10:00 - 10:30	BREAK	BREAK	BREAK	BREAK	BREAK
Chairmen 10:30 - 11:15	<u>W. Thorson</u> W. Lichten	<u>A. Bandrauk</u> R. Marcus	<u>J. Coupe</u> J. Pascale	<u>G. Malli</u> H.F. Schaefer	<u>J. Cizek</u> M. Randic
11:15 - 12:00	W.P. Reinhardt	J.B. Delos	J.N. Bardsley	M. Yoshimine	C.C.J. Roothaan
12:00 - 13:30	LUNCH	LUNCH		LUNCH	LUNCH
Chairmen 13:30 - 14:15	<u>A. Rauk</u> H. Sheraga	<u>D.R. Salahub</u> T. Ziegler	FREE	<u>D. Chong</u> Contributed Papers	<u>R. Boyd</u> Contributed Papers
14:15 - 15:00	J. Kaufman	J.S. Kwiatkowski			
15:00-15:30	BREAK	BREAK		BREAK	
Chairmen 15:30 - 16:15	<u>E. Grein</u> D. McLean	<u>P. Payne</u> K. Morokuma	FOR	<u>B. Sanctuary</u> Contributed Papers	
16:15 - 17:00	P.J. Hay	R. Bartlett E. Davidson	TOURS	<u>T. Dingle</u> Contributed Papers	
17:00 - 19:30	DINNER	DINNER		Business meeting of Canadian Theoretical Chemists	DINNER
19:30 - 20:30	Poster Sessions	Poster Sessions		Barbeque buses leave at 18:30 and 19:00	
21:00 - 22:00	Poster Sessions	Poster Sessions			

Table II. Titles for the Presentations of Invited Speakers

Speaker	Title
Bardsley, J.N. University of Pittsburgh	The Calculation and Use of Optical Potentials
Bartlett, Rodney J. Battelle Columbus Laboratories	Potential Energy Surfaces of Many Body Methods
Bunker, P.R. National Research Council, Ottawa	The Breaking of Molecular Point Group Symmetry
Clarke, B. University of Alberta	How Network Structure Determines the Qualitative Dynamics of Complex Chemical Networks
Davidson, E.R. University of Washington	Some Recent Results on the Long Range Behavior of Wavefunctions
Delos, J.B. FOM Institute, Amsterdam	Electron Detachment in Collisions of Negative Ions with Atoms
Desai, R. University of Toronto	Symmetry Breaking at the Liquid Vapour Interface
Hay, P.J. Los Alamos Scientific Laboratory	Ab Initio Studies of the Structures, Excited States and Reactions of Transition-Metal Complexes Using Effective Core Potentials
Lichten, W. Yale University	Molecular Orbital Model of Atomic Collisions
Kaufman, J. Johns Hopkins University	Ab Initio MODPOT/VRDDO/MERGE Calculations and Electrostatic Molecular Potential Contour Maps
Kwiatkowski, J.S. Nicholas Copernicus University (Poland)	Tautomerism Problem and Environmental Effects on Tautomeric Equilibria
Marcus, R. California Institute of Technology	Energy Randomization in Molecules
Mazenko, G. University of Chicago	Basic Ideas Behind the Renormalization Method in Critical Phenomena

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| McLean, D.
IBM, San Jose | Localized Orbitals in Ab Initio CI Calculations |
| Morokuma, K.
Institute for Molecular
Science (Japan) | Potential Energy Characteristics for Chemical
Reactions |
| Orteleva, P.
Indiana University | Symmetry Breaking and Propagation in Non-
Linear Chemical and Bioelectric Systems |
| Pascale, J.
SRI International | Theoretical Approaches to Collisions of
Rydberg Atoms with Neutrals or Ions |
| Paldus, J.
University of Waterloo | Dynamical Groups: Applications |
| Randic, M.
University of Iowa | Graph Theoretical Approach to Molecular
Structures |
| Reinhardt, W.P.
University of Colorado | Uniform Semiclassical Quantization of
Electronic and Vibrational Motion |
| Roothaan, C.C.J.
University of Chicago | The Quadratically Convergent Multi-Configuration
SCF Method |
| Rossler, O.C.
Universitat Tubingen | Chaos |
| Schaefer III, H.F.
University of California
(Berkeley) | Analytic Configuration Interactions Gradient
Studies of Potential Energy Surfaces |
| Sheraga, H.
Cornell University | Conformational Energy Calculations for
Polypeptides and Proteins |
| Turner, J.S.
University of Texas
(Austin) | Complex Dynamics in Non-Linear Chemical
Systems |
| Umezawa, H.
University of Alberta | A General View of Macroscopic Order and
Disorder in Quantum Many-Body Systems |
| Wulfman, C.E.
University of the Pacific | Symmetry Breaking and Symmetry Retention:
Two Examples |
| Yoshimine, M.
IBM, San Jose | The Symbolic Matrix Method for Expressions of
Matrix Operator's and a Direct CI Procedure
Based on Symbolic Matrices |
| Ziegler, T.
McMaster University | The Calculation of Bond Energies and Bond
Distances by the HFS Transition State Method
Including Relativistic Corrections |

December 29, 1980

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Report to Canadian Theoretical Chemists on the
Seventh Canadian Symposium on Theoretical Chemistry

There were 167 participants, roughly 30% from Canada, 50% from the United States and the balance from locations as far separated as Korea and Greece. Of the participants 37 were students or postdoctoral fellows. The distribution of the invited speakers was similar to that of the participants. There were 29 invited lectures, each of 40 minutes duration, and 95 contributed communications in the form of a 10-minute lecture or a 60-minute poster presentation. It was gratifying that the attendance was excellent to the very end of the Symposium, despite the lure of the surrounding mountains.

The expenses (to the nearest \$100) associated with the symposium were:

1) Invited speakers: ¹	Airfare	\$12,000)	
	Accommodation	4,500)	\$16,500
2) Organization:	Conference Office	3,100)	
	Promotion (printing etc.)	2,700)	6,900
	Poster board, projection	1,100)	
3) Hospitality:	Barbeque	3,600)	
	Reception, coffee etc.	1,700)	6,000
	Transport	700)	
			<u>\$29,400</u>

The income to defray these expenses was generated from:

1) Registrations ²	\$17,400)		
2) Miscellaneous (extra barbeque tickets, transport)	1,000)	\$18,400	
3) Grants:	NSERC	6,500)	
	University of Alberta/		
	University of Calgary	3,600)	11,400
	Other (IBM) etc.	1,300)	
			<u>\$29,800³</u>

¹It should be noted that several invited speakers generously paid their expenses from other sources while yet others accepted only partial payment.

²Registration for invited speakers and session chairmen were waived.

³Actual balance of \$361.05 forwarded for next symposium.

At the organizational meeting held during the Banff symposium André Bandrauk and Russ Boyd agreed to act as co-chairmen for the next meeting to be known, tentatively, as the Eighth International Canadian Symposium on Theoretical Chemistry to be held in 1983 in eastern Canada. Joe Paldus and Ray Kapral were asked to consider chairing the 1986 symposium to be held in Ontario. A slight majority were in favour of holding symposia in resort areas but it was recognized that costs would be a determining factor. It was agreed that the past chairmen and the chairmen for 1983 and 1986 would look into the possibility of a more formal structure although it was generally agreed that the present informal structure had much to recommend it. It was agreed that Vedene Smith's name would be forwarded to the CIC as a contact for the group.

As this concludes our activities as chairmen of the Seventh Canadian Symposium on Theoretical Chemistry we would like to take this opportunity to once again thank all participants, session chairmen and speakers.

S. Huzinaga, Co-chairman
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