

SECOND CANADIAN SYMPOSIUM ON QUANTUM CHEMISTRY

June 26 through June 30, 1967

at the Université de Montréal

Under the auspices of the National Research Council of Canada, and Université de Montréal.

With the financial support of the National Research Council of Canada, Control Data of Canada Ltd., International Bureau Machines of Canada Ltd.

Honorary Committee

A.D. Buckingham, University of Bristol  
R. Daudel, Sorbonne  
R.G. Parr, Johns Hopkins University  
W.G. Schneider, National Research Council of Canada  
O. Sinanoglu, Yale University

Chairmen

C. Sandorfy, Université de Montréal  
M.A. Whitehead, McGill University.

## INFORMATION TO PARTICIPANTS

### Arrival:

There will be no reception committee at the airport.

Airport limousines call at the major downtown hotels but these are still quite far from the University dormitories and you will have to take a cab from the bus terminal.

It is better although somewhat more expensive to take a taxicab at the airport. (about \$5.00). You have to speak to the dispatcher at the exit of the airport building.

Those who will stay at the McGill University residences have to go to: GARDNER HALL, 3935 University Street.

Those who will stay at the Université de Montréal residences have to go to: 2442 Maplewood avenue.

Parking regulations must be strictly observed at both Universities.

Rooms can be occupied from the afternoon of July 25 and have to be vacated by 10 a.m. Sunday, July 2. The rate is \$6.00 a day and you have to pay when you arrive.

### Registration:

There will be registration desks at both the Université de Montréal and McGill University residences open from 2 p.m. until 10 p.m.

Those who chose private accommodation or who arrive late can register on Monday at lunch time in the hall beside the Conference room.

There will be definitely no registration on Monday morning before the inaugural session of the Symposium.

Lectures:

The lectures will take place at room H-415 of the Université de Montréal. Room H-415 is in the main building.

Lectures can be given in english or in french.

Bus service:

There will be a free bus service available between the two Universities.

It will depart from 3935 University Street at 8:15 a.m. on Monday and at 8:30 every day Tuesday through Friday.

In the opposite direction it will depart at 6:00 p.m. from the main entrance of the Université de Montréal every day Monday through Friday.

Ladies' program:

There is a world exhibit on in Montreal. There are wonderful shopping opportunities on St. Catherine Street (Ogilvy's, Simpson's, Eaton's, Morgan's, Dupuis Frères and many smaller stores), at the shopping arcades underneath Place Ville-Marie (the crossshaped skyscraper on Dorchester boulevard) and at many other places.

It is believed that under these circumstances there is no need for a special Ladies' program.

Social events:

Monday evening: Mixer at the Université de Montréal (free)

Thursday evening: 7:00 to 8:00 p.m.: bar available at Gardner Hall, McGill University.

8:00 p.m.: banquet Bishop Mountain Hall, McGill University (\$6.50 inclusive of wine.)

Other details will be given at the Symposium.

Useful telephone numbers:

McGill University residences: 844-6311, ext: 661

Université de Montréal residences: 733-9951, ext: 372

Dr. Whitehead(McGill University): 844-6311, ext: 1210

Dr. Sandorfy(Université de Montréal): 733-9951, ext: 266.

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R. DAUDEL, Sorbonne.  
R.G. PARR, Johns Hopkins University.  
W.G. SCHNEIDER, National Research Council of Canada.  
O. SINANOGLU, Yale University.

CHAIRMEN

- C. SANDORFY, Université de Montréal.  
M.A. WHITEHEAD, McGill University.

PRELIMINARY PROGRAM

Titles listed in the Program are subject to change. Only  
the longer papers are listed. ( 30 or 40 minutes.)

Shorter papers ( 5 or 10 minutes ) will be listed in  
a subsequent circular. Others can be presented by prior agree-  
ment with the chairman of the session.

PROGRAMME

I. Monday, June 26, 1967

a.m. Allocution by Dr. Roger Gaudry, Rector of the Université de Montréal.

- 1) O. SINANOGLU, Yale University, "Prediction of the Stabilities of Molecules by Many-Electron Theory."
- 2) J.A. POPLE, Carnegie Institute of Technology. "Self-Consistent Molecular Orbital Theory for Large Molecules."
- 3) M.J.S. DEWAR, University of Texas "Developments in the SCF MO Theory of Conjugated Molecules."
- 4) Short papers and general discussion.

p.m.

- 1) R. DAUDEL, Sorbonne. "Geminals, bi-orbitals and group-orbitals."
- 2) A.J. COLEMAN, Queen's University. "Geminals, Pure or Applied?"
- 3) Short papers and general discussion.

II. Tuesday, June 27.

- a.m.
- 1) R.G. PARR, Johns Hopkins University. "Accurate Calculations by the One-Center Expansion Method."
  - 2) S.F. BOYS, Cambridge. "The Many Body Problem in Atoms and Molecules."
  - 3) R. PAUNCZ, Technion "Alternant Molecular Orbital Method and the Correlation Problem."
  - 4) Short papers and general discussion.

p.m.      Discussion on Gaussians.

- 1) I.G. CSIZMADIA, University of Toronto.
- 2) B.T. SUTCLIFFE, University of York.
- 3) E. CLEMENTI \* IBM.
- 4) M. KRAUSS, National Bureau of Standards.
- 5) J.W. MOSKOWITZ, New York University.

\* "Exact Computations in Large Molecules."

III.      Wednesday, June 28.

Theory and Experiment.

a.m.

- 1) A.D. BUCKINGHAM, University of Bristol (to be announced)
- 2) E. LIPPERT, Technische Universität Berlin "Theoretical Investigations on the Effect of Induced Emission on the Fluorescence Spectra of Solutions.
- 3) H.O. PRITCHARD, York University, Toronto "Spin Conservation in Chemical Reactions."
- 4) W. SIEBRAND, National Research Council of Canada "Radiationless Transitions in Polyatomic Molecules."
- 5) Short papers and general discussion.

p.m.      free.

IV.      Thursday, June 29.

a.m.

- 1) R. SOMORJAI, National Research Council, of Canada.  
Perturbation-Variation Method for the Calculation of Electron Densities.

- 2) F.W. BIRSS, University of Alberta. "SCF Applications of the Generalized Variational Method."
- 3) S. FRAGA, University of Alberta. "SCF Studies in DNA"
- 4) Short papers and general discussion.

p.m.

- 1) H. HARTMANN, Universität Frankfurt. Title to be announced.
- 2) R.F.W. BADER, Mc Master University, Hamilton. "The Chemical Binding in the First-Row Hydride Molecules."
- 3) Short papers and general discussion.

V. Friday, June 30.

a.m. Valence-Bond Methods.

- 1) J.W. LINNETT, Cambridge.
- 2) M. KARPLUS, Columbia University.
- 3) A. GRIMISON, Universidad de Puerto Rico.

p.m.

- 1) L.C. ALLEN, Princeton University.
- 2) C. ZAULI, Università di Bologna.
- 3) M. SIMONETTA, Università di Milano.



## INFORMATION TO PARTICIPANTS

### I. Accommodation.

Both Mc Gill University and the University of Montreal residences have put 100 single rooms at the disposal of the participants at the rate of \$6 per day ( exclusive of meals).

These rooms can be occupied from the afternoon of Sunday, June 25 and have to be vacated by 10 a.m. Sunday, July 2.

Meals can be taken at the University Cafeterias.

II. The lectures will be held in the main building of the University of Montreal.

Transportation will be available for those participants staying at the Mc Gill University residences which are about 20 minutes from the University of Montreal but closer to downtown Montreal.

III. Registration fee    \$25.00

Graduate students: \$5.00

### IV. Warning.

There will be a World Exhibition on during the Summer of 1967 in Montreal. Therefore hotel reservations have to be made well ahead of time.

If you wish to stay at a hotel in Montreal please make your arrangements through your own travel agent. A partial list of hotels is enclosed.

If you wish to stay at the University residences please return us the enclosed application form within two weeks. We cannot guarantee accommodation to those who fail to do this.

V. Limited attendance.

The total attendance at this symposium cannot exceed 200 due to the facilities available.

VI. Financial help.

To our regret we have no funds to support participants other than those invited speakers needing it.

It is hoped that other participants will be able to provide their expenses from their own travelling grants or from the grant of their professors.

If more funds become available we will let it be known to those who may be interested but at present this seems to be unlikely.