

ALBERTA SYMPOSIUM ON QUANTUM CHEMISTRY

AUGUST 23 - 27, 1965

DIVISION OF THEORETICAL CHEMISTRY
DEPARTMENT OF CHEMISTRY



EDMONTON, ALBERTA
CANADA

November 16, 1964.

Dear Sir:

We are pleased to announce to you the organization of the Alberta Symposium on Quantum Chemistry, which will be held on the campus of the University of Alberta at Edmonton, Alberta, Canada, in the week of August 23- 27, 1965.

It is intended that the Symposium shall last for five days with most of the time given over to invited lectures and discussion, with one or, if necessary, two half days given over to submitted papers.

The emphasis will be mainly upon conventional Quantum Chemistry, including both general theory and chosen applications. The program includes talks on general methods and theories, self-consistent-field theory and applications, problems in correlation, semi-empirical methods and theoretical applications to spectroscopy. The scheduled lecturers will provide an excellent cross-section of the work being carried out at present in Canada, the United States, and Europe. Efforts are being made to obtain contributions from Eastern Europe and the U.S.S.R.

Participants at the Symposium will be lodged at the modern residences of this University, and the meals served in the main Cafeteria. Though we cannot give exact figures at this moment,

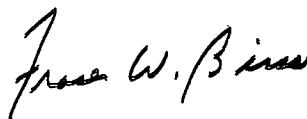
it is expected that the total cost per participant (registration fee and R&B, American style) will be of the order of \$40.00, with \$35.00 being the approximate cost for wives and children older than 12 years. Some time in April of next year we will contact you again with complete details.

Participants who intend to submit short contributions should contact the undersigned at their earliest convenience in order that a tentative program can be set up. It cannot be assured that all the contributions will be accepted, because of lack of time. In this connection it must be pointed out that the contributions should be in line with the general program outlined above. The presentation of last minute contributions will be decided upon at the Symposium by the Chairmen of the different sections, as it is usual in such cases.

We would like also to mention that Edmonton is close to the Canadian Rockies, with the Jasper and Banff National Parks. A summer holiday in sunny Alberta is something to look forward to.

Looking forward to hearing from you and seeing you at the Symposium, we remain

Yours sincerely



Fraser W. Birss



Serafin Fraga



June 22, 1965

Dear Sir

We are sending with this letter information on the Quantum Chemistry Symposium for which arrangements have finally been settled. We would appreciate it if you would bring this to the attention of anyone who might be interested in participating.

Financial arrangements are such that we are able to offer free accommodation to anyone above post-doctoral status, resident in Canada, who otherwise would have to pay these costs himself. For post-doctoral and graduate students in Canada we have funds to offer a limited number of grants to cover accommodation during the Symposium and the fee of \$5. Early notice from those wishing to take advantage of these grants would be much appreciated.

Thank you for your attention,

Yours sincerely

A handwritten signature in cursive script, appearing to read "F. W. Birss".

F. W. Birss

A handwritten signature in cursive script, appearing to read "S. Fraga".

S. Fraga

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DIVISION OF THEORETICAL CHEMISTRY
DEPARTMENT OF CHEMISTRY



EDMONTON, ALBERTA
CANADA

Dear Sir:

We are pleased to present to you the final list of speakers scheduled for the Alberta Symposium on Quantum Chemistry to be held at this University in the week of August 23, 1965.

The lectures will be thirty to forty minutes in length, followed by discussion periods. A variety of topics in general methods and theories in conventional Quantum Chemistry, including self-consistent-field theory and applications, semi-empirical methods, problems in correlation, and applications to spectroscopy, will be covered by these lectures.

We have received a sufficient number of contributed papers to foresee one half-day reserved for submitted papers. If you wish to submit a short contribution please contact the undersigned as soon as possible since the time available will be limited.

Participants at the Symposium will be lodged at the modern residences of this University, and the meals served in the main cafeteria. It is expected that the total cost per participant (registration fee and R & B, American style) will be of the order of \$40.00, with \$35.00 being the approximate cost for wives and children older than 12 years.

In May we will send you a definite program of the scheduled lectures as well as information on travel and alternate accommodation. At that time we will be able to make a definite statement as to the possibility of support for a limited number of participants in the form of free accommodation and meals in the University residences. The funds for the Symposium have been made available by the National Research Council of Canada and the Chemical Institute of Canada.

We will be pleased if you are able to attend.

Yours sincerely,

Fraser W. Birss *Serafin Fraga*
Fraser W. Birss Serafin Fraga

LIST OF SPEAKERS

Tadashi ARAI	Argonne National Laboratory
Paul S. BAGUS	Argonne National Laboratory
Paul E. CADE	L.M.S.S., University of Chicago
A.J. COLEMAN	Queen's University, Kingston
Imre CSIZMADIA	University of Toronto
A. DALGARNO	Queen's University, Belfast
A.A. FROST	Northwestern University
H. HARTMANN	University of Frankfurt
Hugh P. KELLY	University of California, San Diego
Daniel D. KONOWALOW	University of Wisconsin
A.D. McLEAN	IBM Research Laboratory, San Jose
Carl MOSER	Centre de Mecanique Ondulatoire Appliquee, Paris
Robert G. PARR	Johns Hopkins University
Klaus RUEDENBERG	Iowa State University of Science and Technology
Camille SANDORFY	University of Montreal
Charles W. SCHERR	University of Texas
Harrison SHULL	Indiana University
William T. SIMPSON	University of Oregon
Darwin W. SMITH	University of Florida
I. TAMASSY-LENTEI	Kosuth Lajos University, Debrecen
Howard S. TAYLOR	University of Southern California
Arnold C. WAHL	Argonne National Laboratory
Andrew W. WEISS	National Bureau of Standards, Washington

ALBERTA SYMPOSIUM ON QUANTUM CHEMISTRY

University of Alberta, Edmonton, Alberta

Sponsored by the National Research Council of Canada,
The Chemical Institute of Canada and the University of Alberta.

Fraser W. Birss and Serafin Fraga, Co-chairmen

PROGRAMME

MONDAY MORNING

Chairman: C. Sandorfy, Université de Montréal.

- 9:45 Welcoming address by Dr. Max Wyman, Vice-President of the University of Alberta, Edmonton.
- 10:00 A. J. Coleman, Queen's University, Kingston:
"The Density Matrix Approach to the N-Particle Problem".
- 11:00 Coffee
- 11:15 T. Arai, Argonne National Laboratory:
"Cluster Expansion in the Heitler-London Approach to Large Systems".

MONDAY AFTERNOON

Chairman: A. J. Coleman, Queen's University, Kingston.

- 2:00 A. A. Frost, Northwestern University:
"Series Solutions".
- 3:00 Coffee
- 3:15 C. W. Scherr, University of Texas:
"Higher-Order, Perturbation Theory for Excited States"
- 4:15 Coffee
- 4:30 H. W. Taylor, University of Southern California:
"A Proposed Theory of Calculating the Energy of Negative Ion Resonant Elastic Scattering States, and of the Pre-Ionization States of Electronic Spectroscopy".
- 8:30 Mixer: Faculty Club, University Campus.

TUESDAY MORNING

Chairman: W. T. Simpson, University of Oregon.

- 9:00 ~~A. Dalgarno~~^{Taylor}, Queen's University, Belfast:
"Electron Correlation in Atoms".
- 10:00 H. P. Kelly, University of California, San Diego:
"Brueckner-Goldstone Perturbation Theory Applied to Atoms".
- 11:00 Coffee
- 11:15 D. W. Smith, University of Florida:
"Density Matrix Analysis of Wave Functions".

TUESDAY AFTERNOON

Chairman: K. L. McEwen, University of Saskatchewan.

2:00 Contributed Papers:

J. Sokoloff and R. J. Dickson, Research Laboratory, Lockheed Missiles and Space Co., Palo Alto:
"Are the Perturbation Expansions for the Ground State of Neutral Helium the Same for a Hartree Basis Set and a Hartree-Fock Basis Set?".

J. C. Y. Chen, Brookhaven National Laboratory:
"Virtual State Eigenvalue Problems. I. Physical and Mathematical Description".

M. L. Sage and M. D. Girardeau, University of Oregon:
"The Use of Overcomplete Functions in Molecular Calculations".

~~D. W. Howgate~~^{R. Butler}, Solid State Physics Branch, U. S. Missile Command, Redstone Arsenal:
"Green's Function Calculation of Line Shapes of an Interacting Electron-Phonon System".

M. Synek, DePaul University:
"Calculations of Atomic Excited States". (Read)

TUESDAY EVENING

Chairman: R. Bader, McMaster University.

7:15 Contributed Papers:

W. H. Adams, Pennsylvania State University:
"Orbital Theories of Electronic Structure".

I. Shavitt, Israel Institute of Technology:
"Studies in Orbital Optimization".

B. Musulin, M. Povich and C. M. Wang, Southern Illinois University:
"Molecular Screening Parameters".

8:15 Coffee

8:30 Contributed Papers:

S. Rothenberg and E. R. Davidson, University of Washington:
"Hydrogen Molecule Excited States: $1\pi_u$ ".

J. R. Riter, University of Denver:
"The Use of H_2^+ -like Eigenfunctions as Two-Centre Basis Sets
for SCF Calculations".

D. S. Villars, U. S. Naval Ordnance Test Station, China Lake:
"Quantum Mechanics of HO_2 ".

WEDNESDAY MORNING

Chairman: ~~A. Dalgarno~~ ^{Kraus}, Queen's University, Belfast.

9:00 W. T. Simpson University of Oregon:
"Hybridization in Hydrogen Fluoride". (co-author, E. W. Anacker)

10:00 K. Ruedenberg, Iowa State University:
"Localized SCF Molecular Orbitals in Small Molecules".

11:00 Coffee

11:15 A. Weiss, National Bureau of Standards:
"Configuration Interaction in Atoms".

WEDNESDAY AFTERNOON

Chairman: A. A. Frost, Northwestern University.

2:00 R. G. Parr, Johns Hopkins University:
"The Integral Hellmann-Feynman Theorem and its Applications
in Chemistry".

3:00 Coffee

3:15 C. Moser, Centre de Mécanique Ondulatoire Appliquée:
"Rydberg Levels in Diatomic Molecules".

4:15 Coffee

4:30 D. D. Konowalow, University of Wisconsin:
"Quantum Chemistry at Wisconsin"

7:15 Dinner: Faculty Club, University Campus.

THURSDAY MORNING

Chairman: R. G. Parr, Johns Hopkins University.

- 9:00 C. Sandorfy, Université de Montréal:
"Empirical and Semi-Empirical Calculations on Saturated Hydrocarbons".
- 10:00 E. Ruch, Technische Hochschule, München:
"On π -Electron Systems".
- 11:00 Coffee
- 11:15 I. Csizmadia, University of Toronto:
"Gaussian-Type Functions in ab initio Molecular Orbital Calculations".

THURSDAY EVENING

Chairman: I. Csizmadia, University of Toronto.

7:15 Contributed Papers:

G. Berthier, Laboratoire de Chimie Quantique de la Faculté de Sciences de Paris:

" σ and π Radicals in the Series of Nitroxides".

D. Leupold, Deutsche Akademie der Wissenschaften zu Berlin:

"On MO Treatment of the Branching π -Electron Systems". (read)

D. D. Ebbing and L. Poplawski, Wayne State University:

"Some Molecular Calculations on π -Electron Systems Using Geminal Wave Functions".

W. J. Taylor, Ohio State University:

"Hartree-like Approximation to the Fermi Hole in SCF Molecular Orbital Theory: Relation to the Slater and Pariser-Parr-Pople Methods".

8:15 Coffee

8:30 J. F. Harrison, Princeton University:

"Electronic Structure Theory of Polyatomic Molecules: A Gaussian Lobe-Function Approach".

H. F. King, State University of New York, Buffalo:

"A First Order Wave Function for Neon Using Correlated Gaussian Functions".

F. Grein, University of New Brunswick:

"Chemical Shifts and Spin Coupling Constants Calculated from One-Centre Wave Functions".

FRIDAY MORNING

Chairman: K. Ruedenberg, Iowa State University.

- 9:00 P. Bagus, Argonne National Laboratory:
"SCF Excited States".
- 10:00 A. D. McLean, IBM Research Laboratory, San Jose:
"Accurate Wave Functions for Small Molecules: A Clerical Problem".
- 11:00 Coffee
- 11:15 A. C. Wahl, Argonne National Laboratory:
"Hartree-Fock is Here. What next?".