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,~~ Fowler 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".

R. Bader D. W. Howgate, 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 Méchanique 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?".