

THIRD CANADIAN SYMPOSIUM ON THEORETICAL CHEMISTRY

UNIVERSITY OF TORONTO

August 10-16, 1969

SOCIAL EVENTS*

<u>Sunday, August 10</u>	<u>Time</u>	<u>Price per Person</u>
Registrants are invited to the Coffee Party in New College.	6:00 P.M. to	Complimentary
Cold buffet is also available.	11:00 P.M.	\$1.30
<u>Monday, August 11</u>		
President's Reception and Mixer in Hart House.	8:00 P.M.	Complimentary
<u>Wednesday, August 13</u>		
Bus trip to Niagara Falls.	2:00 P.M. [†]	\$3.00
Dinner at the revolving Skylon Tower, overlooking the Falls.		\$6.00
<u>Thursday, August 14</u>		
Co-Chairmen's Reception.	7:00 P.M. [†]	Complimentary
<u>Friday, August 15</u>		
Symposium Banquet in New College. (Bar will be open at 6:30 to 7:30 and 9:30 to 11:30 P.M.)	7:30 P.M.	\$6.00

Other events will be found in the Ladies' Programme.

*Held on the University of Toronto campus, unless otherwise specified.

[†]Times when buses leave New College (Wetmore Hall), 21 Classic Avenue,
University of Toronto campus.

THE THIRD CANADIAN SYMPOSIUM ON THEORETICAL CHEMISTRY

under the auspices of

THE NATIONAL RESEARCH COUNCIL OF CANADA

to be held at

University of Toronto

August 10-16, 1969

HONORARY COMMITTEE:

R. Vaudel, Centre de Mecanique Ondulatoire Appliquée

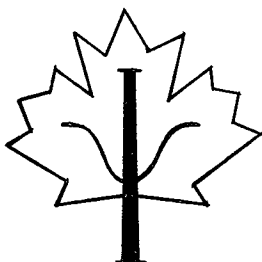
J. Koutecký, Czechoslovak Academy of Sciences
and Visiting Professor at the University of Waterloo

R. G. Parr, Johns Hopkins University

W. G. Schneider, National Research Council of Canada

J. C. Slater, University of Florida
and Massachusetts Institute of Technology

E. B. Wilson, Harvard University



CO-CHAIRMEN:

R. F. W. Bader
McMaster University

I. G. Csizmadia
University of Toronto

Programme

ACKNOWLEDGEMENTS

We express our thanks

to the

UNIVERSITY OF TORONTO

for its hospitality and generous financial support,

and to the

CHEMICAL INSTITUTE OF CANADA.

It is gratefully acknowledged that BELL CANADA, the INTERNATIONAL BUSINESS MACHINES COMPANY LIMITED, and the INTERNATIONAL NICKEL COMPANY OF CANADA LIMITED each sponsored an invited scientist from overseas.

We appreciate the interest shown and the financial support provided by the following members of Canadian Industry:

CANADA PACKERS LIMITED

CONTROL DATA CANADA LIMITED

DUNLOP CANADA LIMITED

DUPONT OF CANADA LIMITED

GULF OIL CANADA

MOLSON'S BREWERY (ONTARIO) LIMITED

ONTARIO HYDRO

THE BRITISH DRUG HOUSES (CANADA) LIMITED

UNION CARBIDE CANADA LIMITED

Finally we, as co-chairmen, are extremely grateful for the assistance of those people, whose names are too numerous to mention, who helped during the organization of this symposium.

MONDAY, AUGUST 11, A.M.

9:00 OPENING ADDRESS: W. G. SCHNEIDER, PRESIDENT, NATIONAL RESEARCH
COUNCIL OF CANADA.

SESSION I

CHAIRMAN: J. C. SLATER, UNIVERSITY OF FLORIDA AND M.I.T.
.....

9:20 S. HUZINAGA, UNIVERSITY OF ALBERTA.

"The coupling operator method in the SCF theory."

10:10 A. T. AMOS, UNIVERSITY OF WATERLOO.

*"Perturbation theory and the generalized eigenvalue
problem."*

M. GIGOU AND M. CORNILLE, LABORATOIRE DE DIFFRACTION
ELECTRONIQUE ET C.M.O.A.

*"Atomic and molecular structure factors in Gaussian
approximation."*

10:30 COFFEE

10:50 L. C. ALLEN, PRINCETON UNIVERSITY.

"Analysis of rotational barriers by means of energy components."

11:40 R. G. PARR, JOHNS HOPKINS UNIVERSITY.

*"On the quantum mechanical virial theorem of molecular
bending motions."*

11:50 A. PULLMAN, UNIVERSITÉ DE PARIS.

*"The image of conjugated molecules in all- and all-valence-
electrons calculations."*

12:40 L. C. SNYDER, BELL TELEPHONE LABORATORIES.

"The electronic structure of thymine."

MONDAY, AUGUST 11, P.M.

SESSION II

CHAIRMAN: D. P. SANTRY, McMASTER UNIVERSITY.
.....

2:00 H. BASCH, FORD MOTOR COMPANY.

"Optical spectra and properties of some organic and inorganic molecules."

2:50 S. D. PEYERIMHOFF, UNIVERSITY OF GIESSEN.

"Structure and spectra of polyatomic molecules in light of recent ab initio MO calculations."

3:40 COFFEE

4:00 J. B. MOFFAT, UNIVERSITY OF WATERLOO.

"Hartree-Fock and the chemical bond."

4:50 D. M. SCHRADER, MARQUETTE UNIVERSITY.

"SCF equations for one-positron, many-electron systems."

K. J. MILLER, RENSSELAER POLYTECH.

"Electron scattering of atoms and molecules for excitations to Rydberg series."

R. P. MESSMER, GENERAL ELECTRIC RESEARCH AND DEVELOPMENT CENTER.

"The optimal overlap variational method: determination of excited state wavefunctions."

J. HORSLEY, LABORATOIRE DE PHOTOPHYSIQUE MOLÉCULAIRE.

"Ab initio calculation of potential surfaces of excited states of H_2O and NH_3 ."

M. L. BENSTON, SIMON FRASER UNIVERSITY.

"Off-diagonal matrix elements by perturbation theory: transition probabilities."

TUESDAY, AUGUST 12, A.M.

SESSION III

CHAIRMAN: J. KOUTECKÝ, CZECHOSLOVAK ACADEMY OF SCIENCES.
.....

9:00 I. SHAVITT, BATTELLE MEMORIAL INSTITUTE AND OHIO STATE UNIVERSITY.

"Configuration interaction calculations for polyatomic systems."

9:50 A. P. JUCYS, THE ACADEMY OF SCIENCES OF LITHUANIAN S.S.R.

"Extended method of calculation and multi-configuration approximation."

10:40 COFFEE

11:00 A. C. WAHL, ARGONNE NATIONAL LABORATORY.

"Correlation energy and its change during molecule formation: numerical results."

11:50 V. H. SMITH, QUEEN'S UNIVERSITY.

"Core polarization and correlation."

TUESDAY, AUGUST 12, P.M.

SESSION IV

CHAIRMAN: H. O. PRITCHARD, YORK UNIVERSITY.
.....

2:00 E. KAPUY, THE HUNGARIAN ACADEMY OF SCIENCES.

"Extended separated pair theory and its application."

2:50 W. KUTZELNIGG, UNIVERSITY OF GÖTTINGEN.

"The numerical treatment of electron correlation in small molecules."

3:40 COFFEE

4:00 H. H. MICHELS, UNITED AIRCRAFT.

"Inverse pre-dissociation in the OH radical--studies of the potential curves."

J. HINZE, UNIVERSITY OF CHICAGO.

"MC-SCF for ground and excited states of diatomics."

D. FU-TAI TUAN, KENT STATE UNIVERSITY.

"Stability of MC-SCF wave function under perturbation."

W. J. TAYLOR, OHIO STATE UNIVERSITY.

"The Hessian matrix in the localization of molecular orbitals."

D. D. EBBING, WAYNE STATE UNIVERSITY.

"Separated electron pair and configuration interaction studies of polyatomic molecules."

H. F. SCHAEFER III, UNIVERSITY OF CALIFORNIA, BERKELEY.

"Symmetry-adapted pair correlations."

A. A. CANTU, UNIVERSITY OF ALBERTA.

"Decomposition of a projected Slater determinant into its valence-bond components."

WEDNESDAY, AUGUST 13, A.M.

SESSION V

CHAIRMAN: S. G. DAVISON, WATERLOO UNIVERSITY.

9:00 N. C. HANDY, JOHNS HOPKINS UNIVERSITY.

"The determination of molecular wave functions with direct inclusion of electron correlation."

9:50 H. CONROY, CARNEGIE-MELLON UNIVERSITY.

"Correlated molecular wave functions."

10:40 COFFEE

11:00 B. T. SUTCLIFFE, UNIVERSITY OF YORK.

"Molecular calculations not making the fixed nucleus approximation."

11:50 P. W. ANDERSON, BELL TELEPHONE LABORATORIES.

"Molecular orbital theory and the chemical bond."

WEDNESDAY, AUGUST 13, P.M.

A trip to Niagara Falls is planned.

THURSDAY, AUGUST 14, A.M.

SESSION VI

CHAIRMAN: A. J. COLEMAN, QUEEN'S UNIVERSITY.
.....

9:00 H. F. HAMEKA, UNIVERSITY OF PENNSYLVANIA.

"The use of Green's functions in atomic and molecular calculations."

9:50 J. P. CARBOTTE, McMASTER UNIVERSITY.

"Pairing correlations in superconductivity."

10:40 COFFEE

11:00 J. PALDUS AND J. CIZEK, UNIVERSITY OF WATERLOO.

"The stability of the Hartree-Fock solutions to electron density fluctuations."

11:50 R. L. SOMORJAI, NATIONAL RESEARCH COUNCIL OF CANADA.

"Integral transform wave functions."

THURSDAY, AUGUST 14, P.M.

SESSION VII

CHAIRMAN: F. W. BIRSS, UNIVERSITY OF ALBERTA.
.....

2:00 H. PRIMAS, SWISS FEDERAL INSTITUTE OF TECHNOLOGY.

"Quantum chemistry in terms of observable quantities."

2:50 R. WALLACE, UNIVERSITY OF MANITOBA.

"Quantum theory of bound systems."

3:40 COFFEE

4:00 H. J. SILVERSTONE, JOHNS HOPKINS UNIVERSITY.

*"On various expansion approaches to the multicenter
integral problem."*

P. VAN LEUVEN, RIJKSUNIVERSITAIR CENTRUM.

*"Use of finite form of spin projection operator in
A.M.O. method."*

E. G. LARSON, UNIVERSITY OF OREGON.

*"The particle-hole matrix of the correlated ground
state, and its connection with the polarizability."*

V. V. KONOWALOW, STATE UNIVERSITY OF NEW YORK AT
BINGHAMTON.

"Zero-S orbitals in molecular problems."

H. A. POHL, OKLAHOMA STATE UNIVERSITY.

"Pseudopotentials in molecules."

V. J. McNAUGHTON AND W. G. HENRY, QUEEN'S UNIVERSITY.

*"A quasi-independent model for atomic structure
calculations."*

FRIDAY, AUGUST 15, A.M.

SESSION VIII

CHAIRMAN: R. G. PARR, JOHNS HOPKINS UNIVERSITY.
.....

9:00 C. MAVROYANNIS, NATIONAL RESEARCH COUNCIL OF CANADA.

"Use of Green's functions in the theory of optical properties of crystals."

9:50 J. LINDERBERG, AARHUS UNIVERSITY.

"Analysis of the electronic correlation problem in molecules and solids."

10:40 COFFEE

11:00 W. SIEBRAND, NATIONAL RESEARCH COUNCIL OF CANADA.

"Electronic-vibrational interactions in aromatic hydrocarbons."

11:50 H. R. FANKHAUSER, MICHIGAN STATE UNIVERSITY.

"On the dynamics of crystals with molecular impurity centers--Green's function approach."

M. R. PHILPOTT, UNIVERSITY OF OREGON.

"Lee models in the theory of molecular excitons and photodissociation reactions."

D. W. HOWGATE, REDSTONE ARSENAL.

"The application of Green's functions and related techniques to a lattice-localized-electron system."

J. CIZEK AND J. PALDUS, UNIVERSITY OF WATERLOO.

"On the use of the Green's function technique for the direct calculation of excitation energies."

S. F. FISCHER, NORTHWESTERN UNIVERSITY.

"The concept of quasi-particles in molecular systems."

P. EMPEDOCLES, UNIVERSITY OF CALIFORNIA.

"Generation of molecular wave functions from those for adjacent nuclear and electronic configurations."

FRIDAY, AUGUST 15, P.M.

SESSION IX

CHAIRMAN: R. F. SNIDER, UNIVERSITY OF BRITISH COLUMBIA.

2:00 J. N. MURRELL, UNIVERSITY OF SUSSEX.

"Some problems in the calculation of intermolecular forces."

2:50 W. J. MEATH, UNIVERSITY OF WESTERN ONTARIO.

"Intermediate and long-range atomic and molecular interactions."

3:40 COFFEE

4:00 O. TAPIA, C.M.O.A.

"Short-range intermolecular forces. SCF LCGO calculation of the H₂--H₂ interaction."

D. LIBERMAN AND J. T. WABER, NORTHWESTERN UNIVERSITY.

"SCF Dirac-Slater calculations for an ion in a dielectric medium."

E. F. HAYES, RICE UNIVERSITY.

"Ring-chain isomerism in three- and four-membered rings."

G. de BROUCKERE, UNILEVER RESEARCH LABORATORY.

"All valence-electron molecular orbital calculations on some transition metal complexes."

V. BELTRAN-LOPEZ, CENTRO NUCLEAR, MEXICO.

"Magnetic moments and spin orbit interaction in the p³ configuration levels of atomic nitrogen."

G. MALLI, SIMON FRASER UNIVERSITY.

"Intra-atomic magnetic interactions in rare-earth atoms."

FRIDAY, AUGUST 15, EVENING.

CONFERENCE BANQUET: SPEAKER - E. B. Wilson, Harvard University.

THE THIRD CANADIAN SYMPOSIUM ON THEORETICAL CHEMISTRY

UNIVERSITY OF TORONTO

AUGUST 10-16, 1969

LIST OF PARTICIPANTS

Aarons, Leon John,
Department of Chemistry,
University of Calgary,
Alberta, Canada.

Amos, A. T.,
Department of Applied Mathematics,
University of Waterloo,
Waterloo, Ontario, Canada.

Anderson, Philip W.,
Bell Telephone Laboratories,
Murray Hill, New Jersey 07974

Anysas, Jurgis A.,
Department of Chemistry,
De Paul University,
Chicago, Illinois 60614

Arents, John,
City College,
Department of Chemistry,
New York, New York 10031

Bader, R. F. W.,
Department of Chemistry,
McMaster University,
Hamilton, Ontario, Canada.

Baird, Norman C.,
Department of Chemistry,
University of Western Ontario,
London, Ontario, Canada.

Basch, Harold,
Theoretical Sciences Department,
Ford Motor Company,
P.O. Box 2058,
Dearborn, Michigan 48121

Beddall, Peter M.,
Department of Chemistry,
McMaster University,
Hamilton, Ontario, Canada.

Beltran-Lopez, Virgilio,
Reactor, Centro Nuclear,
Comision nacional de Energia Nuclear,
Insurgentes sur 1079, Mexico 20, D.F.

Bender, Charles F.,
Battelle Memorial Institute,
505 King Avenue,
Columbus, Ohio 4320

Benesch, Robert,
Department of Chemistry,
Queen's University,
Kingston, Ontario.

Bentley, John,
Carnegie-Mellon University,
Pittsburgh, Pennsylvania 15213

Bertoncini, Peter J.
Argonne National Laboratory,
Argonne, Illinois 60644

Birss, F. W.,
Department of Chemistry,
University of Alberta,
Edmonton, Alberta, Canada.

Blizzard, Alan C.,
Department of Chemistry,
McMaster University,
Hamilton, Ontario, Canada.

Boggs, Joan,
Department of Chemistry,
University of Toronto,
Toronto, Ontario, Canada.

Boyd, D.,
Lilly Research Laboratories,
Indianapolis, Indiana.

Boyd, Russell J.,
Department of Chemistry,
McGill University,
Montreal, Quebec, Canada.

Bukta, Joseph Frank,
1207 Huron Street,
Apartment 203,
London 25, Ontario, Canada.

Brown, Joyce E.,
Department of Chemistry,
Johns Hopkins University,
Baltimore, Maryland 21218

Brown, Richard E.,
Quantum Chemistry Group,
University of Uppsala,
Box 518,
75120 Uppsala 1, Sweden.

Butler, Robert Scott,
Department of Chemistry,
Emory University,
Atlanta, Georgia 30322

Cantu, Antonio A.,
Department of Chemistry,
University of Alberta,
Edmonton, Alberta, Canada.

Cherry, W. H.,
Department of Statistics,
University of Waterloo,
Waterloo, Ontario, Canada.

Chong, Delano P.,
Department of Chemistry,
University of B. C.,
Vancouver 8, B.C., Canada.

Cizek, Jiri,
Department of Applied Maths.,
University of Waterloo,
Waterloo, Ontario, Canada.

Clipsham, Ruth,
Room 429, Otto Maass Bldg.,
McGill University,
Montreal 112, Quebec, Canada.

Cloney, Robert D.,
Department of Chemistry,
Fordham University,
Bronx, New York 10458

Conroy, Harold,
Department of Chemistry,
Carnegie-Mellon University,
Pittsburgh, Pennsylvania 15213

Cooper, I. L.,
Department of Chemistry,
University of Manchester,
Manchester, England.

Cornille, Marguerite,
C.M.O.A.,
23 Rue du Maroc,
Paris, France.

Craft, Lawrence N.,
Department of Chemistry,
University of Pennsylvania,
Philadelphia, Pennsylvania 19104

Csizmadia, I. G.,
Department of Chemistry,
University of Toronto,
Toronto 181, Ontario.

Daiker, K. C.,
Department of Chemistry,
Ohio State University,
Columbus, Ohio.

Davidson, Robert B.,
Frick Chemical Laboratory,
Princeton University,
Princeton, New Jersey 08540

Deal, Ralph M.,
Department of Chemistry,
Kalamazoo College,
Kalamazoo, Michigan 49001

de Brouckere, Guy,
Unilever Research Laboratory,
Vlaardingen, Holland.

de Llano, Carlos R.,
Celanese Chemical Company,
Box 2768,
Corpus Christi, Texas 78403

Desclaux, Jean-Paul,
Commissariat a l'Energie Atomique,
B.P. 27,
94 Villeneuve St. Georges, France.

Ditchfield, Robert,
Mellon Institute,
4400 Fifth Avenue,
Pittsburgh, Pennsylvania 15213

Duben, Anthony J.,
Box 66, Whitmore Laboratory,
Pennsylvania State University,
University Park, Pennsylvania 16802

Durocher, G.,
Department of Chemistry,
University of Montreal,
P.O. Box 6128,
Montreal, Quebec, Canada.

Ebbing, Darrell D.,
105 Old Main,
Wayne State University,
Detroit, Michigan 48202

Empedocles, Philip,
Department of Chemistry,
University of California,
Berkeley, California 94720

Evans, David Keith,
James Frank Institute,
University of Chicago,
5640 S. Ellis Avenue,
Chicago, Illinois 60637

Flurry, Jr., R. L.,
Department of Chemistry,
Louisiana State University at
New Orleans, Louisiana 70122

Fankhauser, Hans R.,
Department of Physics, Michigan
State University,
East Lansing, Michigan 48823

Gangi, Raymond A.,
Department of Chemistry,
McMaster University,
Hamilton, Ontario, Canada.

Gigou, Michele,
Laboratoire de Diffraction Electronique,))) Princeton, New Jersey 08540
Faculte des Sciences,
Orsay, France.

Ginsburg, Jack L.,
Department of Chemistry,
McMaster University,
Hamilton, Ontario.

Grabenstetter, James E.,
Room 329,
Department of Chemistry,
McGill University,
Montreal, 130, Quebec, Canada.

Graves, John L.,
Department of Chemistry,
University of North Carolina,
Greensboro, North Carolina 27412

Hameka, Hendrik F.,
Department of Chemistry,
University of Pennsylvania,
Philadelphia, Pennsylvania 19104

Handy, Nicholas C.,
Department of Chemistry,
The Johns Hopkins University,
Baltimore, Maryland 21218

Harkins, Jerome,
Computer Programming Association Inc.,
P.O. Box 922,
Columbia, Maryland 21043

Hayes, Edward F.,
Department of Chemistry,
Rice University,
Houston, Texas 77001

Hebditch, David,
University of Alberta,
Department of Chemistry,
Edmonton, Alberta, Canada.

Herman, Frank,
IBM Research Laboratories,
Monterey & Cottle Roads,
San Jose, California 95114

Herman, Z. S.,
Department of Chemistry,
Princeton University,
Princeton, New Jersey 08540

Herring, F. Geoffrey,
Department of Chemistry,
University of B. C.,
Vancouver, B.C.

Hinze, Juergen,
Department of Chemistry,
University of Chicago,
Chicago, Illinois 60637

Horsley, John,
Laboratoire de Photophysique Moleculaire,
Batiment 213, Faculte des Sciences,
Orsay, France.

Houlden, Stewart,
Department of Chemistry,
University of Toronto,
Toronto, Ontario, Canada.

Howgate, David W.,
Department of the Army,
Redstone Arsenal, Alabama 35809

Hutchinson, D. A.,
Department of Chemistry,
Queen's University,
Kingston, Ontario.

Huzinaga, Sigeru,
Department of Chemistry,
University of Alberta,
Edmonton, Alberta, Canada.

Ito, Hirotoshi,
Department of Chemistry,
University of Ottawa,
Ottawa, Ontario, Canada.

Jorgensen, W. L.,
Department of Chemistry,
Princeton University,
Princeton, New Jersey 08540

Kaplan, Jerry,
Department of Chemistry,
State University of New York at
Binghamton, New York 13901

Kapral, Raymond,
Department of Chemistry,
University of Toronto,
Toronto, Ontario, Canada.

Kapuy, Ede,
Research Group for Theoretical
Physics,
The Hungarian Academy of Sciences,
XI, Budafoki ut 8, Budapest, Hungary

Kari, Roy,
Department of Chemistry,
University of Toronto,
Toronto, Ontario, Canada.

Kaufman, Joyce J.,
Johns Hopkins University,
Baltimore, Maryland.

King, Frederick W.,
Department of Chemistry,
University of Calgary,
Calgary, Alberta, Canada.

Kollman, Peter Andrew,
Department of Chemistry,
Princeton University,
Princeton, New Jersey 08540

Konowalow, Daniel D.,
Department of Chemistry,
State University of New York at
Binghamton, New York 13903

Koutecky, Jaroslav,
Department of Applied Mathematics,
University of Waterloo,
Waterloo, Ontario, Canada.

Kreek, Holger,
766 Waterloo Street,
London, Ontario, Canada.

Kuppers, B.,
Department of Chemistry,
University of Manitoba,
Winnipeg, Manitoba, Canada.

Kutzelnigg, Werner,
Lehrstuhl für Theoretische Chemie,
34 Göttingen, Bürgerstr. 50a, Germany.

LaForgue, Alex,
University of Lyon,
Lyon, France.

Laidlaw, William G.,
Department of Chemistry,
University of Calgary,
Calgary, Alberta, Canada.

Laing, John R.,
Apt. 8-H, 20 Prince Arthur Avenue,
Toronto 180, Ontario.

Larson, Everett G.,
Department of Chemistry, University of Georgia,
Athens, Georgia 30601

Lawetz, Victor,
Department of Chemistry, Queen's University,
Kingston, Ontario, Canada.

Leffler, Lois C.,
Argonne National Laboratory,
9700 S. Cass Avenue,
Argonne, Illinois 60439

Kekkerkerker, Hendrik N. W.,
Department of Chemistry,
University of Calgary,
Calgary, Alberta, Canada.

Levy, Mel,
Department of Chemistry,
Indiana University,
Bloomington, Indiana 47401

Liang, J. H.,
Ohio State University,
Department of Chemistry,
Columbus, Ohio.

Liebe, Utz,
Department of Chemistry,
University of Alberta,
Edmonton, Alberta, Canada.

Liebman, Joel F.,
Frick Chemical Laboratory,
Princeton University,
Princeton, New Jersey 08540

Lin, C. S.,
Department of Chemistry,
University of Windsor,
Windsor, Ontario, Canada.

Linderberg, Jan,
Department of Chemistry,
Aarhus University,
Aarhus, Denmark.

Lo, Donald H.,
Department of Chemistry,
McGill University,
Montreal, Quebec, Canada.

Macias, Antonio,
Department of Chemistry,
University of Ottawa,
Ottawa, Ontario, Canada.

Malli, Gulzari,
Department of Chemistry,
Simon Fraser University,
Burnaby 2, B.C.

Marchetti, Michael A.,
Department of Chemistry,
Georgetown University,
Washington, D.C. 20007

Mavroyannis, C.,
Division of Pure Chemistry,
National Research Council of Canada,
Sussex Drive,
Ottawa, Ontario, Canada.

McClure, Michael,
Carnegie-Mellon University,
Pittsburgh, Pennsylvania 15213

Meath, W. J.,
Department of Chemistry,
University of Western Ontario,
London, Ontario, Canada.

Mehler, Ernest L.,
Department of Chemistry,
University of Washington,
Seattle, Washington 98105

Messmer, Richard P.,
General Electric Research and Development Center,
Schenectady, New York 12301

Michels, H. Harvey,
Department of Physics,
United Aircraft Research Laboratories,
East Hartford, Connecticut 06108

Michl, Josef,
Department of Chemistry,
Aarhus University,
Aarhus, Denmark.

Miller, Kenneth J.,
101 Walker, Department of Chemistry,
Rensselaer Polytech. Institute,
Troy, New York 12181

Moffat, John B.,
Department of Chemistry,
University of Waterloo,
Waterloo, Ontario, Canada.

Morokuma, Keiji,
Department of Chemistry,
University of Rochester,
Rochester, New York 14627

Moscowitz, A.,
Department of Chemistry,
University of Minnesota,
Minneapolis, Minnesota 55455

Moseley, David,
Department of Chemistry,
Washington State University,
Pullman, Washington 99163

Munn, R. W.,
Division of Chemistry,
National Research Council of Canada,
Sussex Drive, Ottawa 7, Ontario, Canada.

Murrell, John N.,
Chemical Laboratory,
University of Sussex,
Brighton, Sussex, England.

Neumann, David B.,
Bell Telephone Laboratories,
Room 1a364,
Murray Hill, New Jersey 07974

Nieuwpoort, W. C.,
Department of Chemistry,
University of Groningen,
The Netherlands.

O'Shea, James F.,
Department of Chemistry,
McMaster University,
Hamilton, Ontario.

Paldus, Joseph,
Quantum Theory Group,
Department of Applied Mathes.,
University of Waterloo, Ontario,
Canada.

Parr, Robert G.,
Department of Chemistry,
Johns Hopkins University,
Baltimore, Maryland 21218

Pelletier, Jocelyn,
Department of Chemistry,
McMaster University,
Hamilton, Ontario, Canada.

Peyerimhoff, Sigrid D.
Institut für Theoretische Physik,
Justus Liebig Universität,
63 Giessen, Lahn, Leihgesterner Weg,
Germany.

Pfeiffer, Gary V.
Department of Chemistry,
Ohio State University,
Athens, Ohio 45701

Philpott, Michael R.,
Institute of Theoretical Science,
University of Oregon,
Eugene, Oregon.

Pipano, Aharon,
Battelle Memorial Institute,
505 King Avenue, Columbus, Ohio.

Pohl, Herbert A.
Department of Physics,
Oklahoma State University,
Stillwater, Oklahoma 74074

Popkie, Herbert,
LMSS, Department of Physics,
University of Chicago,
Chicago, Illinois 60637

Primas, Hans,
Swiss Federal Institute of Technology,
Physical Chemistry Laboratory,
Universitatstr. 22,
8006 Zurich, Switzerland.

Pritchard, H. O.,
CRESS, York University,
Downsview, Ontario, Canada.

Pullman, Alberte,
Institut de Biologie Physico-Chimique,
13, Rue Pierre Curie,
Paris 5, France.

Raas, E. Richard,
25 Kennedy Blvd.,
East Brunswick, New Jersey 08816

Rauk, Arvi,
Frick Chemical Laboratories,
Princeton University,
Princeton, New Jersey 08540

Robb, Mike,
Department of Chemistry,
University of Toronto,
Toronto, Ontario.

Rosen, Philip,
Hasbrouck Laboratory,
University of Massachusetts,
Amherst, Massachusetts 01002

Rothenberg, Stephen,
University Computing Company,
260 Sheridan Avenue, Palo Alto,
California 94306

Rouse, Robert A.,
Department of Chemistry,
Harvard University,
Cambridge, Massachusetts 02138

Rumble, John,
Department of Chemistry,
Indiana University,
Bloomington, Indiana 47401

Runtz, Gordon,
Department of Chemistry,
McMaster University,
Hamilton, Ontario.

Russell, Anthony W.,
Memorial University,
(Junior Division),
St. John's, Newfoundland.

Sachs, Lester M.,
Computer Programming Association,
P.O. Box 922,
Columbia, Maryland 21043

Sack, Robert Arno,
Department of Mathematics,
University of Salford, England.

Salahub, Dennis Russell,
Department of Chemistry,
University of Montreal,
Montreal, Quebec.

Sanctuary, Bryan C.,
Department of Chemistry,
University of B.C.,
Vancouver 8, B.C.

Sanderson, Barry A.,
Department of Chemistry,
State University of New York,
Buffalo, New York 14214

Santiago, Maria,
Carnegie-Mellon University,
Pittsburgh, Pennsylvania 15213

Santiago, Sue,
Department of Chemistry,
University of Toronto,
Toronto, Ontario.

Santry, D. P.,
Department of Chemistry,
McMaster University,
Hamilton, Ontario.

Schachtschneider, Jerry,
Shell Development Company,
Emeryville, California 94608

Schaefer, Henry F.,
Department of Chemistry,
University of California,
Berkeley, California 94720

Scherr, Sister Virginia,
Department of Chemistry,
Louisiana State University,
Baton Rouge, Louisiana 70302

Schmid, G. H.,
Department of Chemistry,
University of Toronto,
Toronto, Ontario, Canada.

Schneider, W. G.,
President, National Research Council of Canada
100 Sussex Drive, Ottawa 7, Ontario.

Schoenborn, Mike,
Department of Chemistry,
University of Toronto,
Toronto, Ontario.

Schrader, David M.,
Department of Chemistry,
Marquette University,
Milwaukee, Wisconsin 53233

Shavitt, Isaiah,
Battelle Memorial Institute,
505 King Avenue,
Columbus, Ohio 43201

Shupack, Saul I.,
Department of Chemistry,
Villanova University,
Villanova, Pennsylvania 19085

Siebrand, W.,
Division of Pure Chemistry,
National Research Council of Canada,
Sussex Drive,
Ottawa 7, Ontario, Canada.

Silver, David M.,
Department of Chemistry, Harvard University,
Cambridge, Massachusetts 02138

Silverstone, Harris J.,
Department of Chemistry,
Johns Hopkins University,
Baltimore, Maryland 21218

Slater, John C.,
Quantum Theory Project, Nuclear Science Bldg.,
University of Florida, Gainesville, Florida.

Slezak, Jane A.,
Department of Chemistry,
University of Pittsburgh,
Pittsburgh, Pennsylvania 15213

Smith, Jr., Vedene H.,
Department of Chemistry,
Gordon Hall, Queen's University,
Kingston, Ontario, Canada.

Snider, Robert F.,
Department of Chemistry,
University of B.C.,
Vancouver 8, B.C.

Snyder, Lawrence C.,
Bell Telephone Laboratories,
Murray Hill, New Jersey 07974

Somorjai, R. L.,
Division of Pure Chemistry,
National Research Council of Canada,
Sussex Drive, Ottawa 7,
Ontario, Canada.

Stauffer, A. D.,
CRSSS, York University,
Downsview, Ontario.

Stevens, Richard M.,
Harvard University,
Cambridge, Massachusetts 02138

Stevens, Walter, J.,
Department of Chemistry,
Box 278,
Indiana University,
Bloomington, Indiana 47401

Sutcliffe, Brian T.,
Department of Chemistry,
University of York,
Heslington, York, England.

Sutton, P. W.,
North Central College,
Department of Physics,
Naperville, Illinois 60540

Tapia, Orlando,
C.M.O.A.,
23 Rue du Maroc,
Paris 19, France.

Taylor, W. J.,
Ohio State University,
Columbus, Ohio.

Tel, Luis,
Department of Chemistry,
University of Toronto,
Toronto, Ontario.

Thomas, Michael W.,
Department of Chemistry,
University of B. C.,
Vancouver 8, B. C.

Tomasi, Jacopo,
Istituto di Chimica Fisica,
Universita di Pisa,
Via del Risorgimento 35,
56100 Pisa, Italy.

Tseng, Tien-Jiunn,
Department of Chemistry,
University of New Brunswick,
Fredericton, N.B.

Tu, Rem-Sing,
Department of Chemistry,
University of New Brunswick,
Fredericton, N.B.

Tuan, Debbie F.,
Department of Chemistry,
Kent State University,
Kent, Ohio. 44240

Van Leuven, Piet,
Department of Theoretical Physics,
Rijksuniversitair Centrum,
Middelheimlaan 1,
Antwerpen, Belgium.

Vasudevan, Kris,
Department of Chemistry,
University of Calgary,
Calgary 44, Alberta, Canada.

Veguilla-Berdecia, Luis A.,
Department of Chemistry,
American University,
Washington, D.C.

Voigt, Bjorn,
Kemisk Institut,
Aarhus Universitet,
Vangelaudsgade,
8000 Aarhus C., Denmark.

Waber, James T.,
Department of Chemistry,
Northwestern University,
Evanston, Illinois 60201

Wahl, Arnold C.,
Division of Chemistry,
Argonne National Laboratory,
Argonne, Illinois 60439

Wallace, R.,
Department of Chemistry,
University of Manitoba,
Winnipeg, Manitoba.

Weltin, Eugene E.,
Department of Chemistry,
University of Vermont,
Burlington, Vermont 05401

Womack, Jr., Cahvus M.,
Department of Chemistry,
Texas Southern University,
Houston, Texas 77004

Wright, James S.,
Laboratoire de Chimie Theorique,
Batiment 496,
Faculte Des Sciences,
Orsay, France.

Wu, A. A.,
Department of Chemistry,
University of Ottawa,
Ottawa, Ontario, Canada.

Yue, C. P.,
Department of Chemistry,
University of B.C.,
Vancouver 8, B.C.

Zeiss, Geoffrey,
Department of Chemistry,
McGill University,
Montreal, Quebec.

Baranovsky, S.C.,
Division of Chemistry,
National Research Council of Canada,
Ottawa 7, Ontario.

Peat, David,
National Research Council of Canada,
Ottawa, Ontario.

Carbotte, J. P.,
Department of Physics,
McMaster University,
Hamilton, Ontario.

Davison, Sydney G.,
Department of Applied Maths.,
University of Waterloo,
Waterloo, Ontario.

Coleman, A. J.,
Department of Mathematics,
Queen's University,
Kingston, Ontario, Canada.

Wilson, E. B.,
Harvard University,
Cambridge, Massachusetts.

THIRD CANADIAN SYMPOSIUM ON THEORETICAL CHEMISTRY

UNIVERSITY OF TORONTO

August 10-16, 1969

SOCIAL EVENTS*

<u>Sunday, August 10</u>	<u>Time</u>	<u>Price per Person</u>
Registrants are invited to the Coffee Party in New College.	6:00 P.M. to	Complimentary
Cold buffet is also available.	11:00 P.M.	\$1.30
<u>Monday, August 11</u>		
President's Reception and Mixer in Hart House.	8:00 P.M.	Complimentary
<u>Wednesday, August 13</u>		
Bus trip to Niagara Falls.	2:00 P.M. [†]	\$3.00
Dinner at the revolving Skylon Tower, overlooking the Falls.		\$6.00
<u>Thursday, August 14</u>		
Co-Chairmen's Reception.	7:00 P.M. [†]	Complimentary
<u>Friday, August 15</u>		
Symposium Banquet in New College. (Bar will be open at 6:30 to 7:30 and 9:30 to 11:30 P.M.)	7:30 P.M.	\$6.00

Other events will be found in the Ladies' Programme.

*Held on the University of Toronto campus, unless otherwise specified.

[†]Times when buses leave New College (Wetmore Hall), 21 Classic Avenue,
University of Toronto campus.