THE SIXTH CANADIAN SYMPOSIUM ON THEORETICAL CHEMISTRY UNIVERSITY OF NEW BRUNSWICK 19-25 JUNE 1977

HONORARY COMMITTEE

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J. C. Polanyi	(University of Toronto)
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O. K. Rice	(University of North Carolina)
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CO-CHAIRMEN

W. Forst	(Université Laval)
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SPONSORS

National Research Council of Canada

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GENERAL INFORMATION FOR PARTICIPANTS

Badges

Please wear your Symposium badge at all times. It serves as identification for use of the lecture rooms, recreational facilities, the Faculty Club, and for the complimentary social events.

Information Desk

The information desk in the lobby of MacLaggan Hall will be open on

Monday from	8:00 A.M. - 12:00 NOON
Tuesday to Saturday	8:15 A.M. - 10:30 A.M.

Food and Bar Services

Food will be served in the cafeteria on the ground floor of the Student Union Building (No. 34 on campus map), or in the Faculty Club on the third floor of the Old Arts Building (No. 18 on campus map). A temporary membership card for the Faculty Club is enclosed in your registration kit.

Since special arrangements were made for an earlier opening time of the cafeteria, it will be appreciated if participants would take their breakfast in the cafeteria.

The opening times are as follows:

Cafeteria:		
Breakfast	Monday	8:00 - 9:30
	Tuesday - Saturday	7:30 - 9:30
Lunch	Monday-Friday	11:30 - 13:30
Dinner	Monday,Wednesday,Friday	16:45 - 18:15
	Tuesday,Thursday	16:45 - 18:00
Faculty Club		
Breakfast	Monday-Friday	8:00 - 10:00
Lunch	Monday-Friday	12:00 - 14:00

On Saturday and Sunday the Coffee Shop, also located on the ground floor of the Student Union Building, will be open from 10:00 - 18:00.

A list of restaurants in the Fredericton area is attached.

Bar services will be available in the Faculty Club during the times

Monday-Friday	11:30 - 1:00 A.M.
Saturday	20:00 - 1:00 A.M.

Social Events

Dean's Mixer on Sunday, 19 June, from 19:00 - 23:00, in the Memorial Student Centre (No. 30 on campus may). This mixer is partly sponsored by the Dean of Science, and is complimentary.

Picnic on Tuesday, 21 June, at the Mactaquac Provincial Park. Buses will be waiting in the parking lot opposite Mackenzie House (No. 40 on campus map), and will leave at 14:00. They are scheduled to return around 19:00. The Picnic is part of the social events' package and tickets will be required.

Lobster Dinner on Thursday, 23 June, in the dining room of Lady Dunn Hall (No.45 on campus map). Fresh boiled lobster will be served from 18:00 to 19:00. The lobster dinner is part of the social events' package, and tickets will be required.

Concert on Thursday, 23 June, at 20:30 in Memorial Hall (No. 27 on on campus map). A string concert, lasting for about 1/2 hour, will be performed by the Resident Musicians. Please be on time! The concert is complimentary.

President's Reception, immediately following the concert, in the Memorial Student Centre. This reception is partly sponsored by the President of this University, and will be complimentary for all participants and their spouses.

Lecture Rooms

All lectures will be held in MacLaggan Hall (No. 35 on campus map). All invited, and most of the contributed papers, will be given in the auditorium, room 105. Room 16 of MacLaggan Hall will always be available for people to relax and talk.

Notice to Speakers

A slide projector for 35 mm slides and an overhead projector with an acetate roll will be available. A limited number of transparencies can be obtained at the information desk. Due to the large number of contributions, the lecture (plus discussion) time for communications will have to be restricted to 10 minutes.

Notice to Canadian Participants

A meeting to discuss the future of the Canadian Symposia on Theoretical Chemistry will take place on Wednesday, 22 June, at 13:30 in room 14 of MacLaggan Hall.

Mail and Telephone Messages

Mail can be obtained at the information desk, or in room 15 of F.J. Toole Hall (No. 22 on campus map, opposite MacLaggan Hall).

Telephone messages can be left at the Chemistry Department, Tel.(506)453-4781.

Parking

Free parking is permitted in all parking zones on the U.N.B. campus.

Use of Chemistry and Science Libraries

All participants are welcome to use the facilities of the Chemistry Library, located in Room 107 of F.J. Toole Hall (No. 22 on campus map), and of the Science Library in the Integrated University Complex (No. 21b on campus map), containing the Physics collection.

Recreational Facilities

All recreational facilities of U.N.B. will be available free of charge to Symposium participants and their families. However, the Symposium badge will be required as identification. Family members may obtain a badge at the information desk.

Sir Max Aitken Swimming Pool in Lady Beaverbrook Gymnasium (No.28 on campus map)

Casual Swims (no children)	Monday to Friday	11:30-13:30 P.M.
	Monday to Friday	17:30-18:30 P.M.
	Monday to Thursday	21:30-22:30 P.M.
	Friday	18:30-21:00 P.M.
	Saturday	15:00-17:00 P.M.
Family Swims (children under 16 to be accompanied by parents)	Wednesday	19:30-20:30 P.M.
	Saturday	19:30-21:00 P.M.
	Sunday	14:00-16:00 P.M.

Lady Beaverbrook Gymnasium

Hours open:	Monday-Saturday	8:00 - 22:30 P.M.
	Sundays	12:30 - 17:30 P.M.

For handball, squash and paddleball please book courts in advance at 453-4578.

Shuffle board courts: Located on the patio between Tibbits and Lady Dunn Hall.

Horse Shoe Pits: Located on the up hill side of the Residence Office Building.

The Alumni Tennis Courts: Located on the up hill side of Lady Dunn Hall.

SELECTED LIST OF RESTAURANTS

China House Restaurant - Fully licensed - 454-6042
Dining Room
136 Prospect Street

The Coffee Mill Burgundy Room - Fully licensed - 454-9996
Fredericton Shopping Mall
Prospect Street
Seafood and Steaks

The Condor Motor Lodge Restaurant - 455-5537
Woodstock Road
Seafood and Canadian Foods

The Cosmo Club - 454-9180
Dining Room - Gourmet Foods
Steak House
524 King Street (Please make reservations)

Diplomat Motor Inn - Fully Licensed - 454-6489
Dining Room and Lounge
225 Woodstock Road
Canadian and Chinese Foods
Seafood and Steaks
Chinese Buffet at noon daily.

Dragon City Dining Room - Fully licensed - 455-6695
Dining Room and Cabaret
151 Westmoreland Street (downtown Fredericton)
Exotic Chinese Dishes, Steaks and Seafood

Keddy's Motor Inn - Fully licensed - 454-4461
Forest Hill Road

Lord Beaverbrook Hotel - Fully licensed - 455-3371
Dining Room and
Maverick Room (specializing in Steaks)

Moon Palace - Fully licensed - 454-2494
Lincoln Road
Specializing in Exotic Chinese Dishes

Sea Esta Seafood Restaurant - Fully licensed - 472-3986
274 Main Street
Steaks and Seafood

Voyageur Restaurant - Fully licensed - 454-3908
Trans Canada Highway West

Wandlyn Motor Inn - Fully licensed - 455-8937
58 Prospect Street

Restaurants for the Family

A&W Drive-In 454-9259
1180 Smythe Street

Capital Gardens 455-8331
558 Queen Street (downtown Fredericton)
Chinese and Canadian dishes

The Coffee Mill Family Restaurant 454-9996
Fredericton Shopping Mall
Prospect Street

The Dairy Queen 472-7861
525 Union Street

Frank's Foods 454-2246
Exhibition Park
Smythe Street

Harvey's 455-6484
460 Regent Street

House of Hay - Kentucky Fried Chicken 455-9997
81 Regent Street
Prospect Street

McDonald's 454-6830
Prospect Street

Mother Marten's Restaurant 454-1661
King's Place
King Street (downtown Fredericton)

The Ponderosa Steak House 454-9095
Prospect Street

Pizza Nova 454-6627
74 York Street

Tim Horton
Prospect Street

Restaurants - Delivery

Dixie Lee Fried Chicken 454-2177
Also Pizza

Luna Pizza - Pizza and other Italian Food 455-4020
298 King Street

Pizza Delight 455-5206
254 King Street

THE SIXTH CANADIAN SYMPOSIUM
ON THEORETICAL CHEMISTRY

UNIVERSITY OF NEW BRUNSWICK, FREDERICTON, N.B.
19-25 June 1977

SCIENTIFIC PROGRAMME

All lectures will be held in the auditorium (room 105),
or in rooms 14 and 18 of MacLaggan Hall.

Monday 20 June 1977

9:00-10:00	F. Grein and W. Forst	Chairmen
Room 105	President's Welcome	
35 Min.	R. S. Mulliken U. Chicago	THE NATURE OF CHEMICAL BONDING
10:30-12:30	E. R. Davidson	Chairman
Room 105 35 Min.	I. Shavitt BattelleColumbus Labs.	STATUS REPORT ON CONFIGURATION INTERACTION
35 Min.	W. Meyer U. Kaiserlautern	ELECTRON CORRELATION BY THE METHOD OF SELF-CONSISTENT ELECTRON PAIRS
10 Min.	K. Tanaka,M. Yoshimine IBM Research Lab.	THEORETICAL STUDY ON THE ISOMERS OF THE SYSTEM C_2H_2 + O
10 Min.	N.H.Sabelli, M, Kantor, T. L. Gilbert, A. C. Wahl U. of Illinois	CALCULATION OF POTENTIAL CURVES FOR THE SHORT RANGE HIGHLY REPULSIVE REGION: A&H and A&H$^+$
14:15-15:45	R. F. Snider	Chairman
Room 105 40 Min.	J.C. Polanyi U. of Toronto	THEORIES OF 'MACROSCOPIC BRANCHING' (ALTERNATIVE REACTION PRODUCTS) AND 'MICROSCOPIC BRANCHING' (ALTERNATIVE REACTION DYNAMICS)
35 Min.	H. Hartmann U. Frankfurt	THEORY OF BIMOLECULAR COMPENSATION EFFECTS
16:15-17:45		
Room 105	B. C. Eu	Chairman
35 Min.	J. Ross MIT	CHEMICAL INSTABILITIES
35 Min.	R. Lefever U. Libre de Bruxelles	RECENT PROGRESS IN DISSIPATIVE STRUCTURES AND FLUCTUATION THEORY
20:00-21:30		
Room 105	F. W. Birss	Chairman
10 Min.	D. P. Chong U. British Col.	PREDICTION OF LARGE CORRECTIONS TO KOOPMANS' THEOREM
10 Min.	K. Helfrich U. Berlin	AB INITIO EXTENSION OF MULLIKEN'S DEMI-H_2^+-MODEL APPLIED TO EXCITED STATES OF H_2 AND He_2.
10 Min.	C. F. Jackels BattelleColumbus Labs.	POTENTIAL ENERGY SURFACE STUDY OF THE TWO LOWEST-LYING EXCITED STATES OF THE H_2O^+ ION.
10 Min.	R. Kari Laurentian Univ.	MINIMAL BASIS SET LOCALIZED MOLECULAR ORBITALS
10 Min.	L. Lawlor, F. Grein, K. Vasudevan U. New Brunswick	AB INITIO STUDIES ON THE ELECTRONIC STRUCTURE OF ONF (NITROSYL FLUORIDE)

10 Min.	P. C. McKinney Wabash College	THE FUNCTIONS ASSOCIATED WITH THE BURRAU APPROXIMATION FOR THE HYDROGEN MOLECULAR ION AND ANALOGOUS MOLECULES EXPRESSED AS CONTINUED FRACTIONS
10 Min.	L. E. Nitsche,E.R.Davidson U. Washington	THE $^1\pi\pi^*$ STATE OF FORMAMIDE CALCULATED FROM PERTURBATION THEORY
10 Min.	J. Sichel,J. Langlois U. Moncton	COUPLING OF ANGULAR MOMENTA IN DOUBLY EXCITED STATES OF NEON
21:40 Room 105	D. P. Chong	Chairman
10 Min.	D. M. Silver Johns Hopkins U.	INTERACTION POTENTIALS BETWEEN CLOSED-SHELL ATOMS AND MOLECULES
10 Min.	K. Vasudevan, F. Grein U. New Brunswick	ELECTRON AFFINITY OF C_2H
10 Min.	S. Wilson Inst.for Space Studies	DIAGRAMMATIC PERTURBATION EXPANSION APPLIED TO THE CARBON MONOSULPHIDE MOLECULE
10 Min.	A. Gupta, R.J. Boyd Dalhousie U.	ELECTRON CORRELATION AND THE ELECTRON DENSITY OF ATOMS AND MOLECULES
10 Min.	W. Woznicki Copernicus U.	CORRELATION EFFECTS IN LITHIUM ISOELECTRONIC SEQUENCE
10 Min.	R. J. Blint G.M. Technical Center	A POTENTIAL ENERGY DESCRIPTION OF THE HYDROGEN ATOM PLUS OXYGEN MOLECULE REACTIONS
10 Min.	S. L. Guberman Center for Astrophysics	AB INITIO POTENTIAL CURVES FOR ADIABATIC AND DIABATIC STATES OF O_2
10 Min.	H. B. Jansen Free U. Amsterdam	NEW DEVELOPMENTS IN THE CALCULATION OF NUCLEAR SPIN-SPIN COUPLING CONSTANTS
10 Min.	B.D.Joshi,K.Morokuma State U. New York	AB INITIO CALCULATIONS AND ANALYSES OF ENERGIES AND FORCES ALONG THE INTRINSIC REACTION COORDINATE
10 Min.	S. Nagase,K. Morokuma U. Rochester	AB INITIO MO STUDY OF ORGANIC REACTIONS.ENERGY, CHARGE, AND FORCE DECOMPOSITION ANALYSES

Tuesday 21 June 1977

8:30-10:00 Room 105	B. Sanctuary	Chairman
35 Min.	R. F. Snider U. Brit. Col.	OBSERVABLES, OPERATORS AND COLLISIONS
35 Min.	R. Wallace U. Manitoba	ITERATIVE METHODS IN THE THEORY OF MOLECULAR PROCESSES
10:30-12:30 Room 105	A. C. Wahl	Chairman
35 Min.	K. Ruedenberg Iowa State Univ.	DESCRIPTION OF CHEMICAL REACTIONS IN A FULL-OPTIMIZED REACTION SPACE
35 Min.	B. Roos U. Stockholm	DIRECT CONFIGURATION INTERACTION METHODS AND THEIR APPLICATION TO MOLECULAR STRUCTURE CALCULATIONS AND CHEMICAL REACTIONS

10 Min.	T. H. Dunning Los Alamos Scientific Labs.	POTENTIAL ENERGY SURFACES FOR ABSTRACTION AND EXCHANGE IN H + HCl
10 Min.	K.E.Banyard,J.C.Moore and C. E. Reed U. Leicester	ANGULAR AND RADIAL CORRELATION EFFECTS IN MOMENTUM SPACE FOR H^-, He and Li^+
14:00	P I C N I C	Buses to leave at 14:00 from MacKenzie House
20:00-21:30 Room 105	L. C. Snyder	Chairman
35 Min.	J. J. Kaufman Johns Hopkins U.	THEORETICAL AND QUANTUM CHEMICAL APPROACHES TO QUANTUM PHARMACOLOGY AND QUANTUM BIOLOGY
35 Min.	A. Veillard U. Louis Pasteur	OXYGEN BINDING TO METALLOPORPHYRINS
21:40 Room 105	POSTER SESSION R. J. Boyd	Chairman
	B.G.Adams,J. Paldus U. Waterloo	ATOMIC CORRELATION PROBLEM: COUPLED CLUSTER APPROACH
	L. A. Curtiss Argonne Nat. Lab	AB INITIO MOLECULAR ORBITAL STUDIES OF SMALL CLUSTERS OF WATER AND METHANOL MOLECULES
	R.D. Harcourt Cornell U.	"INCREASED-VALENCE" STRUCTURES FOR ELECTRON-EXCESS SYSTEMS
	J. L. Ginsburg St. Mary's U.	SENSITIVITY OF INTERSTELLAR CH AND CH^+ ABUNDANCES TO H_2 PHOTODISSOCIATION MODELS
	P. J. Hay Los Alamos Sci. Lab.	ELECTRONIC STATES OF $CR(CO)_5$ FROM AB INITIO SCF AND CI CALCULATIONS
	F. H. Mies National Bureau of Standards	A SCATTERING THEORY OF DIATOMIC MOLECULES USING DIABATIC ELECTRONIC-ROTATIONAL STATES
	R. R. Gamache U. Massachusetts	THE THEORY OF MOLECULAR DEFECTS IN CRYSTALS AND SMALL MOLECULES TRAPPED IN MATRICES
	C. Petrongolo Lab.Quant.Chem.	AB INITIO SCF STUDY OF PAIR INTERACTION BETWEEN GLYCINE AND SERINE ZWITTER-IONS AND WATER
	E. L. Mehler U. Basel	SELF-CONSISTENT NON-ORTHOGONAL GROUP FUNCTION APPROXIMATION FOR POLYATOMIC SYSTEMS
	S. Swaminathan, D. L. Beveridge Hunter College	A THEORETICAL STUDY OF A DILUTE AQUEOUS SOLUTION OF METHANE
	D.H.Phillips,R.Raffenetti, E.R. Long, Jr. NASA	IONIZATION POTENTIALS AND CATION DISSOCIATION ENERGIES OF H_2O and $(H_2O)_2$
	C. Trindle,E.A.Halevi U. Virginia	APPLICATION OF ORBITAL CORRESPONDENCE ANALYSIS IN MAXIMUM SYMMETRY (OCAMS) TO SPIN-FORBIDDEN PROCESSES
	R. C. Raffenetti Argonne National Lab.	A SIMULTANEOUS RELAXATION METHOD FOR CONFIGURATION INTERACTION EXCITED STATE EIGEN PROBLEMS
	D. F. Tuan,G.W. Loar Kent State U.	SCF $X\alpha$ SW METHOD WITH OVERLAPPING SPHERES

	Y.G. Smeyers Lab.Quant.Chem.-Spain	COMPARISON BETWEEN THE HALF-PROJECTED AND PROJECTED HARTREE-FOCK SCHEMES
	A. Wagner,A.C.Wahl, A. Karo,P.Krejci Argonne Nat. Lab.	CLASSICAL INELASTIC SCATTERING IN LiH_2: A COMPARISON OF DIFFERENT POTENTIAL ENERGY SURFACES

Wednesday June 22, 1977

8:30-10:00 Room 105	M. Zerner	Chairman
40 Min.	A. Pullman U. Paris	RECENT DEVELOPMENTS IN QUANTUM BIOLOGY
35 Min.	P. Kollman U. California	THEORETICAL STUDIES OF SMALL MOLECULE-LARGE MOLECULE INTERACTIONS
10:30-12:30 Room 105	J. Paldus	Chairman
35 Min.	J. Cizek U. Waterloo	ON THE USE OF ALGEBRAIC METHODS FOR THE CALCULATION OF LONG-RANGE MOLECULAR FORCES
35 Min.	I. G. Csizmadia U. Toronto	THE BORN-OPPENHEIMER ENERGY PARTITIONING AND ITS STEREOCHEMICAL CONSEQUENCES
10 Min.	M. Randic Iowa State U.	ON THE PROBLEM OF SUBGRAPH ISOMORPHISM (OR SEARCHING FOR PARTICULAR FRAGMENTS IN A STRUCTURE
10 Min.	J. Goodisman Syracuse U.	CALCULATION OF THE SURFACE TENSION OF A MOLTEN SALT
14:15-15:45 Room 105	T. Carrington	Chairman
35 Min.	W. A. Lester IBM	NON-ADIABATIC ASPECTS OF COLLISIONAL ENERGY TRANSFER
35 Min.	J. C. Tully Bell Labs.	ELECTRONICALLY NON-ADIABATIC CHEMICAL REACTIONS
16:15-17:45 Room 105	W. Siebrand	Chairman
35 Min.	J. C. Lorquet U. Liege	NON-ADIABATIC INTERACTION IN UNIMOLECULAR DECAY
35 Min.	W. Thorson U. Alberta	NON-ADIABATIC COUPLINGS DONE CORRECTLY
20:00-21:30	PANEL DISCUSSION:	CONFIGURATIVE INTERACTION AND ITS IMPACT ON THEORETICAL CHEMISTRY
	I. Shavitt	Chairman
	E. R. Davidson U. Washington	
	W. Meyer U. Kaiserslautern	
	S. D. Peyerimhoff U. Bonn	

	B. Roos U. Stockholm	
	A. C. Wahl Science Applications	
21:40 Room 14	J. Sichel	Chairman
10 Min.	S.Y.Chang,H.Weinstein Ebasco Services, Inc.	ADDITIVITY IN THE PERTURBATION TREATMENT OF MULTIPLE SITE REACTIVITY IN LARGE MOLECULES
10 Min.	M.P.S.Collins,M.C.Zerner U. Guelph	A COMPLETE NEGLECT OF DIFFERENTIAL DIATOMIC OVERLAP THEORY
10 Min.	O. Noell,K.Morokuma U.Rochester	AN AB INITIO INVESTIGATION OF THE RELATIVE STABILITY OF BENT AND LINEAR COORDINATION OF THE NITROSYL LIGAND IN $Co(NH_3)_5NO^{+2}$
10 Min.	L. C. Snyder Bell Laboratories	THE HYDROGEN BONDS OF UREA IN UREA CRYSTAL AND WITH WATER
10 Min.	K. Weiss, J.I.Scott Northeastern U.	AB INITIO CALCULATIONS ON Π-MOLECULAR COMPLEXES
10 Min.	W.H.Adams, E. E. Polymeropoulos Rutgers Univ.	APPLICATION OF THE LOCALIZED-WAVE-FUNCTION EXCHANGE-PERTURBATION-THEORY TO H_2^+ AND H_2
10 Min.	D. L. Freeman U. Rhode Island	COUPLED-PAIR MANY-ELECTRON THEORY APPLIED TO EXTENDED ELECTRONIC SYSTEMS
10 Min.	O. Gropen U. Alberta	SCF MODEL POTENTIAL CALCULATIONS ON METAL COMPLEXES
10 Min.	H. J. Monkhorst U. Utah	APPLICATION OF COUPLED-CLUSTER METHOD TO OPEN-SHELL SYSTEMS
10 Min.	G. H. Loew Stanford U.	AB INITIO CALCULATIONS OF CANDIDATE INTERSTELLAR MOLECULES: HNCO, HOCN, HCNO AND HONC
TITLE	S. Guha Saha Inst.,Calcutta	THE CONFORMATIONAL PROPERTIES OF PHENYLEPHRINE (FREE BASE) BY MOLECULAR ORBITAL TECHNIQUE
TITLE	G. A.Henderson Southern Illinois U.	ORBITALS FOR HIGHLY CORRELATED ELECTRON DENSITIES: THE HELIUM GROUND STATE
21:40 Room 18	D. R. Salahub	Chairman
10 Min.	J. M. Bowman, K.T. Lee Illinois Inst. of Tech.	SUDDEN ROTATION REACTIVE SCATTERING CALCULATIONS OF THE 3-D H + H_2 REACTION
10 Min.	A.Komornicki,K.Morokuma and T. F. George NASA	SEMICLASSICAL DYNAMICS ON MULTIPLE ELECTRONIC SURFACES: THREE-DIMENSIONAL QUASICLASSICAL TREATMENT OF REACTIVE F + H_2 AND F + D_2
10 Min.	P. J. Kuntz Hahn Meitner Inst.	CURVE-CROSSING PROCESSES IN THE IONIC SYSTEMS $NeHe_2^+$ AND FH_2^+
10 Min.	P. Mezey U. Toronto	TRANSITION STATE DETERMINATION BY THE X-METHOD
10 Min.	A. Penner, W. Forst National Research Council	RELAXATION AND DECOMPOSITION IN A THERMAL SYSTEM WITH EXPONENTIAL TRANSITION PROBABILITIES

10 Min.	N. Sathyamurthy,J.C.Polanyi U. Toronto	A CLASSICAL TRAJECTORY STUDY OF ROTATIONAL ENERGY TRANSFER IN HCL + M (M=Ar, He,HCl) COLLISIONS
10 Min.	A. E. Foti Queen's U.	ELECTRONIC CONFIGURATION AND MOLECULAR STRUCTURE OF S_n
10 Min.	D.R.Salahub,R.P.Messmer U. Montreal	THEORETICAL STUDIES OF THE CHEMISORPTION OF OXYGEN ATOMS ON ALUMINUM
10 Min.	D. J. Klein U. Texas	LOCALIZED-SITE CLUSTER EXPANSIONS FOR MOLECULAR AND SOLID-STATE WAVEFUNCTIONS
10 Min.	M. Steslicka U. Waterloo	SURFACE STATES: ARE THEY IMPORTANT IN FIELD IONIZATION
TITLE	H. F. Hameka U. Pennsylvania	CALCULATION OF NON LINEAR ELECTRIC POLARIZABILITIES
TITLE	N. S. Snider Queen's U.	TEMPERATURE VARIATION OF RATE CONSTANTS FOR ATOM RECOMBINATION

Thursday June 23, 1977

8:30-10:00 Room 105	N. S. Snider	Chairman
35 Min.	W. H. Miller U. California	RECENT DEVELOPMENTS IN SEMI-CLASSICAL SCATTERING THEORY
35 Min.	A. Bandrauk U. Sherbrooke	A SCATTERING THEORY APPROACH TO PRE-DISSOCIATION
10:30-12:30 Room 105	G. Hunter	Chairman
35 Min.	R. T. Pack Los Alamos Sci. Lab.	ANGULAR MOMENTUM DECOUPLING APPROXIMATIONS IN MOLECULAR SCATTERING THEORY: HOW TO MAKE A HARD PROBLEM EASY
35 Min.	H. K. Shin U. Nevada	VIBRATIONAL ENERGY TRANSFER
10 Min.	K. Kay, R.W. Numrich Kansas State U.	COMPUTATIONAL STUDIES OF DISSOCIATION DYNAMICS IN MODEL COLLINEAR TRIATOMIC SYSTEMS
10 Min.	C. S. Sloane Oakland U.	HYDROGEN ADDITION TO ETHYLENE
14:15-15:45 Room 105	H.F. Hameka	Chairman
35 Min.	O. Goscinski U. Uppsala	TRANSITION OPERATORS AND PROPAGATORS
35 Min.	M. A. Whitehead McGill U.	Xα AND ALL THAT: THEORY, PROBLEMS, IMPROVEMENTS AND RESULTS
16:15-17:45 Room 105	J. E. Harriman	Chairman
35 Min.	R.F.W. Bader McMaster U.	THE QUANTUM DEFINITION OF AN ATOM IN A MOLECULE - A THEORETICAL BASIS FOR DESCRIPTIVE CHEMISTRY
35 Min.	A. Hardisson U. La Laguna	ABSORPTION LINE SHAPE OF TWO COUPLED OSCILLATORS

18:00 LOBSTER DINNER IN LADY DUNN HALL

20:30 CONCERT IN MEMORIAL HALL FOLLOWED BY

RECEPTION IN MEMORIAL STUDENT CENTRE

Friday 24 June 1977

8:30-10:00 Room 105	K. Weiss	Chairman
40 Min.	C. Sandorfy U. Montreal	RYDBERG STATES IN PHOTOCHEMICAL REACTIONS
35 Min.	K. F. Freed U. Chicago	PHOTOCHEMICAL REACTION DYNAMICS IN POLYATOMIC SYSTEMS
10:30-12:30 Room 105	G. Diercksen	Chairman
35 Min.	D. A. Ramsay NRC	RECENT SPECTROSCOPIC STUDIES OF THEORETICAL INTEREST
35 Min.	S. D. Peyerimhoff U. Bonn	CONFIGURATION INTERACTION CALCULATIONS FOR MOLECULAR SPECTRA: VALENCE AND RYDBERG STATES AND INFLUENCE OF VIBRATIONS
10 Min.	D.L. Yeager, M. Herman and K. F. Freed U. Chicago	ANALYSIS OF THIRD ORDER CONTRIBUTIONS TO EQUATIONS OF MOTION-GREEN'S FUNCTION IONIZATION POTENTIALS: APPLICATION TO N_2
10 Min.	A.C. Albrecht Cornell U.	RAMAN SCATTERING OF BENZENE IN THE UNTRAVIOLET: THEORY AND EXPERIMENT
14:15-15:45 Room 105	B. Widom	Chairman
40 Min.	O. K. Rice U. North Carolina	INTERFACIAL TENSION NEAR THE CRITICAL POINT: SOME NEW ASPECTS AND RELATIONSHIPS
35 Min.	B. I. Halperin Harvard Univ.	THEORY OF DYNAMIC CRITICAL PHENOMENA
16:15-17:45 Room 105	O. K. Rice	Chairman
35 Min.	J.M.H.Levelt Sengers Nat. Bureau of Standards	UNIVERSALITY OF CRITICAL BEHAVIOR
35 Min.	B. Widom Cornell U.	THREE-PHASE EQUILIBRIA AND TRICRITICAL POINTS
20:00-21:30 Room 14	R. Kari	Chairman
10 Min.	D.L.Beveridge,S.Swaminathan Hunter College	A THEORETICAL STUDY OF THE STRUCTURE OF LIQUID WATER BASED ON QUASICOMPONENT DISTRIBUTION FUNCTIONS
10 Min.	M. Mezel,D.L. Beveridge Hunter College	MONTE CARLO STUDIES OF DILUTE AQUEOUS SOLUTIONS OF THE K^+ AND F^- IONS

10 Min.	P. Brumer,J.W.Duff U.Toronto	STATISTICAL BEHAVIOR AND EXPONENTIAL INSTABILITY IN COLLINEAR ATOM-DIATOM COLLISIONS
10 Min.	B. C. Eu McGill U.	ASYMPTOTIC SOLUTIONS OF FOKKER-PLANCK EQUATIONS AND GENERALIZED ONSAGER-MACHLUP THEORY
10 Min.	I. Absar, A.J. Coleman Queen's U.	OPTIMAL ORBITAL BASIS SETS FOR THE MANY-ELECTRON PROBLEM
10 Min.	T. Carrington York U.	THE REPRESENTATIONS OF COMMUTING OPERATORS
10 Min.	W. H. Fink U. California	TAKING ADVANTAGE OF LOCAL SYMMETRY
10 Min.	G. Grenet, M. Kibler U. Lyon	IRREDUCIBLE TENSOR METHODS AROUND LIGAND FIELD THEORY. APPLICATION TO Eu^{3+} IN TETRAGONAL SYMMETRY
20:00-21:30 Room 18	T. W. Dingle	Chairman
10 Min.	R. N. Camp Brandeis U.	CALCULATION OF STRUCTURE FACTORS FOR VALENCE ELECTRON DENSITIES
10 Min.	S.R.Langhoff,J.O.Arnold, R.L.Jaffe & D.M.Cooper NASA	THEORETICAL STUDY OF MOLECULES OF INTEREST TO JUPITER ENTRY
10 Min.	J.R.LaVega Villanova U.	SYMMETRY AND TUNNELLING IN PROTON TRANSFER REACTIONS
10 Min.	H. D. Todd Wesleyan U.	EXPLICIT REPRESENTATION OF LONE-PAIR ELECTRON DENSITY IN MOLECULAR WAVEFUNCTIONS
10 Min.	E. Ludena, M. Zuvia Inst. Venezolano	CHARGE DISTRIBUTION ANALYSIS IN TERMS OF BERLIN'S BINDING AND ANTIBINDING REGIONS FOR Li_2 AND F_2
10 Min.	C. Zauli, D.P.Craig, P.Palmieri and P. Stiles U. Bologna	CIRCULAR DICHROISM IN SPIRO [4,4] NONATETRAENE
21:40 Room 105	J. L. Ginsburg	Chairman
10 Min.	P. W. Payne U.North Carolina	ELIMINATION OF EXCHANGE ENERGY FROM HARTREE-FOCK THEORY
10 Min.	W. J. Taylor Ohio State U.	INVERSE GAUSSIAN TRANSFORMS: GENERAL PROPERTIES AND APPLICATION TO SLATER-TYPE ORBITALS WITH NON-INTEGER AND INTEGER n IN THE COORDINATE AND MOMENTUM REPRESENTATION
10 Min.	E. W. Abrahamson,M.P.S.Collins, K. Kear and S. Khandelwal U. Guelph	ELECTRONIC ENERGY TRANSFER IN SMALL MOLECULES IN THE GAS PHASE
10 Min.	R.L.Jaffe,S.R.Langhoff NASA	PHOTODISSOCIATION OF TRIATOMIC MOLECULES IN THE STRATOSPHERE: APPLICATION TO HOCl AND HO_2
10 Min.	T. D. Bouman Southern Illinois Univ.	OPTICAL ACTIVITY CALCULATIONS IN THE RANDOM PHASE APPROXIMATION

10 Min.	E. G. Larson Brigham Young Univ.	REDUCED TRANSITION DENSITY MATRICES AND OSCILLATC STRENGTHS FOR TRANSITIONS OF THE 4-ELECTRON BORON ION B+"
10 Min.	H. Johansen Techn. Univ. Denmark	AB INITIO SCF AND CI CALCULATION OF THE PHOTO-ELECTRON SPECTRUM OF COBALT OXIDE
10 Min.	J. Grabenstetter, R.J. LeRoy Univ. Waterloo	ON THE BOUND LEVELS AND POTENTIAL ENERGY SURFACE OF THE HCl-Ar VAN DER WAALS COMPLEX
10 Min.	A. J. Thakkar Univ. Waterloo	THE INTRAMOLECULAR BOND LENGTH DEPENDENCE OF THE ANISOTROPIC DISPERSION COEFFICIENTS FOR HYDROGEN MOLECULE-NOBLE GAS OR ALKALI ATOM INTERACTIONS
10 Min.	H. J. Silverstone, T. Yamabe, and A. Tachibana Johns Hopkins Univ.	ON THE FIELD IONIZATION OF THE HYDROGEN ATOM

SATURDAY, JUNE 25, 1977

8:30-10:00 Room 105	M. A. Whitehead	Chairman
35 Min.	J. Simons Univ. Utah	SPECTRA AND MIGRATION OF EXCESS ELECTRONS IN CONDENSED MEDIA
35 Min.	G. Wolken, Jr. Battelle Inst.	DYNAMICS OF HETEROGENEOUS REACTIONS: GAS SOLID COLLISIONS
10:30-12:00 Room 105	D. L. Beveridge	Chairman
35 Min.	E. Clementi Montedison Res. Inst.	QUANTUM CHEMISTRY AND STATISTICAL MECHANICS IN COMPLEX CHEMICAL SYSTEMS: CONFORMATIONAL ANALYSES AND SOLVENT EFFECTS
35 Min.	V.H. Smith, Jr. Queen's Univ.	WHAT'S NEW IN DENSITY MATRICES: A REPORT FROM THE MONCTON CONFERENCE