

LIST OF PARTICIPANTS

Dr. A. Amirav
School of Chemistry
Tel-Aviv University
Tel-Aviv 69978
ISRAEL

Dr. O. Bohigas
Institut de Physique Nucléaire
Université Paris-Sud
91405 Orsay
France

Prof. Mark Child
Theoretical Chemistry Department
1 South Parks Road
Oxford OX1 3TG
England

Dr. Nguyen Dang
Faculté des Sciences
Université de Sherbrooke
Sherbrooke, Québec J1K 2R1
Canada

Dr. W. Dietz
Technische Universität München
Institut für Theoretische Physik T38
D-8046 Garching,
West Germany

Prof. W. Domcke
Institute of Physical and Theoretical
Chemistry
Technical University of Munich
D-8046 Garching
West Germany

Dr. M. Dupré
Service National des Champs Intenses
du CNRS
BP 166X
38042 Grenoble Cedex
France

Dr. Stavros Farantos
Department of Chemistry
University of Crete
and
Institute of Electronic Structure and Laser
Research Center of Crete
711 10 Iraklion, Crete
Greece

Prof. S. Fischer
Technische Universität München
Institut für Theoretische Physik T38
D-8046 Garching
West Germany

Prof. R. B. Gerber
Fritz Haber Center for Molecular Dynamics
and
Department of Physical Chemistry
Hebrew University
Jerusalem
Israel

Prof. Maximo Garcia-Sucre
Instituto Venezolano de Investigaciones
Científicas
and
Universidad Central de Venezuela
Caracas
Venezuela

Prof. James T. Hynes
Department of Chemistry and Biochemistry
University of Colorado
Boulder, Col. 80309
U. S. A.

Dr. R. Jost
Service National des Champs Intenses
du CNRS
BP 166 X
38042 Grenoble Cedex
France

Prof. Jan Kommandeur
Laboratory for Physical Chemistry
The University of Groningen
Nijenborgh 16
9747 AG GRONINGEN
The Netherlands

Dr. Sydney Leach
Laboratoire de Photophysique Moléculaire
du CNRS
Université Paris-Sud
91405 Orsay
France

Prof. Roland Lefebvre
Laboratoire de Photophysique Moléculaire
du CNRS
Université Paris-Sud
91405 Orsay
France

Prof. Donald H. Levy
James Franck Institute
and Department of Chemistry
University of Chicago
Chicago, Ill. 60637
U. S. A.

Dr. M. Lombardi
Service National des Champs Intenses
du CNRS
BP 166 X
38042 Grenoble Cedex
France

Dr. Giorgio Mantica
Dipartimento di Fisica
Università di Milano
Milano
Italy

Prof. William Miller
Department of Chemistry
University of California
and
Materials and Molecular Research Division
Lawrence Berkeley Laboratory
Berkeley, Cal. 94720
U. S. A.

Prof. C. B. Moore
Department of Chemistry
University of Berkely
Berkeley, Cal. 94720
U. S. A.

Prof. Shaul Mukamel
Department of Chemistry
University of Rochester
Rochester, N. .Y. 14627
U. S. A.

Dr. P. Papagiannakopoulos
Department of Chemistry
University of Crete
and
Institute of Electronic Structure and Laser
Research Center of Crete
711 10 Iraklion, Crete
Greece

Prof. Charles S. Parmenter
Department of Chemistry
Indiana University
Bloomington, Ind. 47405
U. S. A.

Prof. Mark A. Ratner
Department of Chemistry
Northwestern University
Evanston, Ill. 60201
U. S. A.

Prof. E. Riedle
Institut für Physikalische und
Theoretische Chemie
Technische Universität München
Lichtenbergstr. 4
D-8046 Garching
West Germany

Prof. Israel Schek
Department of Chemistry
and Institute for Theoretical Chemistry
University of Texas
Austin, Texas 78712
U. S. A.

Dr. Benoit Soep
Laboratoire de Photophysique Moléculaire
du CNRS
Université Paris-Sud
91405 Orsay
France

Prof. H. S. Taylor
Department of Chemistry
University of Southern California
Los Angeles, Cal. 90089
U. S. A.

Dr. André Tramer
Laboratoire de Photophysique Moléculaire
du CNRS
Université Paris-Sud
91405 Orsay
France

Prof. Veronica Valda
Department of Chemistry and Biochemistry
University of Colorado
Boulder, Col. 80309
U. S. A.

SUBJECT INDEX

A

Absorption spectrum, *see* CS₂, OCS, NH₃
Action spectrum, 158-159
Adiabatic switching method, 82
Adiabatic angular eigenvalues, 246
Alkyl benzene, 163
Anderson localization, 6
Anharmonic interactions, 193
Anthracene, 172
 absolute fluorescence quantum yield, 173-174
 absorption spectrum of, 173
 fluorescence excitation spectrum of, 173-174
Atom migration, 242
Attractor, 17
Autocorrelation function, 222, 228

B

Bath, 263
Benzene, 171, 193, 203, 273
 cation, 223, 227, 228
Billiards, 2
Born Oppenheimer separation, 23
Bound-free emission, 155, 156
Brody distribution, 33, 66, 68

C

Channel three, 203
Chaos, 1, 15-29
 classical, 1, 16
 quantum, 1, 16, 31, 48
 vibrational, 24
Chemical timing, 164
Chirikov resonance, 4
CH₃I, 254
Classical equations of motion, 236
Clusters, 233-243
 fragmentation dynamics, 237-239
CO₂, 76
Conformer, 141
Conical intersection, 217, 218

- Coordinates
 - hyperspherical, 61, 245
 - local, 60
 - normal, 60
 - reaction, 245, 263
- Coriolis coupling, see vibronic interaction
- Correlation diagram, 249-251
- Coupling model, 193
- CS₂, 253, 254-256
 - absorption spectrum, 255

D

- Dark states, 177, 194
- Decay
 - behavior of individual levels, 209
 - multiple exponential, 177, 180
 - non exponential, 175
 - non radiative (ultrafast), 217
 - radiative, see lifetime
- Degrees of freedom
 - rotational 171
- Δ_3 statistic of Dyson and Mehta, 46
- Density of vibrational states, 137
- Dephasing contributions, 177
- Diabatic potentials, 219
- Dissociation
 - remote bond, 279
- Doorway states, 175
- Doppler-free excitation, 203-204

E

- Einstein-Brillouin-Keller quantization, 81
- Electronic relaxation
 - interstate, 171, 175
- Energy localization, 274
- Energy redistribution, 133, 137
 - dynamics of 163, 164
 - intramolecular vibrational, 163, 171
 - lifetime of 163, 164
 - rotational effect in vibrational..., 171
- Entropy, generalized, 195
- Ethylene cation, 222
- Exciplex state, 133
 - interaction, 143
 - intermolecular, 140
 - intramolecular, 140

F

Fermi resonance, see Resonance
Fluctuation measures, 46
Fluorescence excitation spectrum,
 see anthracene,
 HgN₂, HgH₂, 9-cyanoanthracene
 Infra-red, 163, 164
Fokker-Planck equation, 4
Free rotors, 236

G

Gaussian
 orthogonal ensemble, 21, 31, 46
 thawed, 114, 197
 unitary ensemble, 21
 wavepackets, 109, 113

H

H₃⁺, 245
Half-collisions, 157
HCN, 25, 62, 72, 73
HDO, 71
Hénon-Helles potential, see potential
H₂O, 59
Homogeneous linewidths, 200, 254
Hydrogen atoms, 1
 Rydberg, 2
Hydrogen peroxide H₂O₂, 273, 276
HgH₂, 149
 fluorescence excitation spectrum, 159
HgN₂, 149
 fluorescence excitation spectrum, 150-151, 154
Hyperspherical coordinates, see coordinates

I

Impurity molecule, 234
Initial preparation, 96
Interference effects, 177
Intermediate sized molecules, 171
Internal conversion, 175
 rotation, 164
Irregular spacings, 255
Isomerization, 62, 273

J

Jahn-Teller effect, 218, 225

K

K. A. M. theorem, 3, 16, 54

KCN, 21

Kolmogorov entropy, 19, 50

L

Langevin equations generalised, 263, 264

Laser excitation

of a multi-mode system, 99

Level repulsion, 47

Libration, 153, 235

LICN, 21

Lifetime

broadening, 279

radiative, 175, 176, 217

RRKM, 278

Linewidth

homogeneous, 264

inhomogeneous, 279

Liouville operator, 110

classical, 113

Lyapunov functions, 19

M

Matrices

real symmetric random, 31

Methyl group, 163

substitution, 163

rotor, 164, 165

Mixing property, 49

Mode localization, 23

Molecular beam, 134, 149, 171, 185

Multi-mode phenomenon, 217

Multiphoton excitation, 99

N

Nearest neighbor spacing, 20

NH₃, 253, 257-259

absorption spectrum, 258

- Nodal structure, 20
- Nonradiative decay, 203
- 9-cyanoanthracene, 172, 177
 - absolute fluorescence quantum yield of, 178-179
 - absorption spectrum of, 178-179
 - fluorescence excitation spectrum, 178-179
- Nuclear exchange, 245

O

- O₃, 25, 254
- OCS, 253, 256-257
 - absorption spectrum, 256
- Onset of stochasticity, 25
- Oscillators
 - non linearly coupled, 85
- Overtone reaction, 273-281

P

- Padé procedure, 127
- p-difluorobenzene, 163
- Perturbation
 - complex, 130
 - spectroscopic, 254
- p-fluorotoluene, 163
- Photodissociation dynamics, 31-41, 235, 257, 263, 276
- Photoelectron spectrum, 223, 226
- Photofragment spectroscopy, 259
- Phthalocyanine, 137
- Poincaré surfaces of section, 19
- Poisson distribution, 66
 - spectrum, 47
 - statistics, 31
- Potential
 - adiabatic, 27
 - Hénon-Helles, 16, 93
 - optical, 127
- Power spectrum, 19
- Predissociating molecules, 253-260
- Pyrazine, 171, 182, 185
 - quantum yield of fluorescence, 190
 - rotational spectrum of, 189

Q

- Quantum beats, 177

- Quantum localization, 2, 4, 5
- Quantum stability, 10
- Quantum yield of fluorescence, 172, 179, 186, 187
 - see also anthracene, 9-cyanoanthracene, pyrazine
- Quasiperiodicity, 15

R

- Radiationless transitions, 171
- Raman excitation profiles, 115, 119, 120
- Random coupling model, 99
- Random matrices ensembles, 2, 45
- Random matrices theory, 46
- Rate of exponential divergence, 19, 21
- Reactive flux correlation function, 263, 269
- Recursive residue generation method 96
- Regime
 - chaotic, 95
 - classical chaotic, 95
 - quasiperiodic, 95
- REMPI (resonance enhanced multiphoton ionization), 134, 141
- Renner-Teller splitting, 256
- Resolution of the rotational structure, 193
- Resonance
 - Fermi, 88, 96, 273, 274, 277
 - non linear, 273
 - overlapping, 65
 - quantum resonance states, 123
 - Raman, 259
 - string of, 131
- Rotation
 - complex, 124
- Rotational distribution, 161
- Rotor-vibrational level, 165, 166
- RRKM (Rice, Ramsperger, Kassel and Marcus)
237, 276, 279, 281

S

- Schrödinger equation, 265
- Self-consistent field approximation, 59
 - semi-classical, 57-80
 - time dependent, 64, 109, 265
- Sensitivity of eigenvalues to small perturbations, 20
- Separatrix, 84
- Shock wave, 239
- Siegert wave, 127

Solid matrices, 233-243
Spectral congestion, 255
Spectral fluctuations, 45
Spectral rigidity, 37, 52
SSH theory, 167
Stadium potential, 16
Stark effect
 radial, 128
Supersonic jets, 193
Survival probability, 96, 98, 101-106

T

Time dependent description, 221, 228
 see also self-consistent time dependent.
Trajectory
 chaotic, 21
 classical, 237
 quasiperiodic, 21, 69
Transition
 from regular to irregular states, 16
Transition state theory, 276
Triatomics, 17
Truncation effects, 41
Tryptophan, 134
Tunnelling, 62
 proton, 146
 reaction, 243

U

Uniform semi-classical quantization, 63
Unimolecular process, 253

V

Vague torus, 91
Van der Waals complexes, 149-161
 interaction, 163
 rotor-vibration energy transfer, 168
Vibrational crossing, 183
Vibrational predissociation, 245
Vibrational relaxation, 217
 state mixing, 165
Vibronic interaction
 anharmonic, 175
 Coriolis, 175, 180, 181, 182, 185, 188, 193,
 208-213

W**Wigner distribution, 66****Z****Zwitterion, 133, 143**