Sunday, 28 September

Session 1	Chair: Martin Quack, ETH Zürich
19:30 – 20:15	Jürgen Troe, Göttingen Reaction Dynamics with Wavepackets, Adiabatic Channels and Classical Trajectories
20:15 – 21:00	Martin Jungen, Basel What is a muon doing in atoms or molecules ?

Monday, 29 September

Session 2	Chair: Werner Kutzelnigg, Bochum
08:30 – 09:15	Wim Klopper, Karlsruhe Explicitly correlated calculations of excitation energies
09:15 – 10:00	David Luckhaus, Göttingen Direct Multi-Arrangement Quantum Dynamics: From Vibrations to Reactions
10:00 – 10:30	Coffee Break
Session 3	Chair: Peter Botschwina, Göttingen
10:30 – 11:15	John P. Maier, Basel Electronic Spectroscopy of Carbon Chains and Such: Relevance to Astrophysics and Nanoscience
11:15 – 12:00	Frédéric Merkt, ETH Zürich High-Resolution VUV Spectroscopy, Rydberg States and Cations
12:00 – 14:00	Lunch Break
Session 4	Chair: Wilfried Meyer, Kaiserslautern
14:00 – 14:45	Hans-Joachim Werner, Stuttgart Explicitly correlated local wavefunctions: LMP2-R12 with density fitting
14:45 – 15:30	Jeppe Olsen, Aarhus Coupled Cluster Expansions with Quadruple and Higher Excitations
15:30 – 16:00	Coffee Break
Session 5	Chair: Jürgen Hinze, Bielefeld
16:00 – 16:45	Gernot Frenking, Marburg The Nature of the Chemical Bond - Old Questions, New Answers
16:45 – 17:30	Kimihiko Hirao, Tokyo (PCCP Lecture) Recent advances in electronic structure theory
18:00 – 19:30	Dinner Break
	Mounting of Posters
19:30 – 22:00	Poster Session (EVEN numbered)

Tuesday, 30 September

Session 6	Chair: Walter Thiel, Mülheim
08:30 – 09:15	N.N. (Hellmann Prize)
09:15 – 10:00	Tom Rizzo, Lausanne State-resolved molecule surface reactions - a challenge for theoreticians
10:00 – 10:30	Coffee Break
Session 7	Chair: Hans-Peter Lüthi, ETH Zürich
10:30 – 11:15	Roberto Marquardt, Marne-la-Vallée Vibrational and Rotational Wave Packet Motion in Polyatomic Molecular Systems
11:15 – 12:00	Regina de Vivie-Riedle, München Analysis and coherent control of ultrafast molecular processes
12:00 – 14:00	Lunch Break
	Afternoon: Posters / Discussions / Free / Excursion
19:00	BBQ Dinner

Wednesday, 1 October

Session 8	Chair: Dirk Schwarzer, Göttingen
08:30 – 09:15	Sam Leutwyler, Berne Excited-state H-atom transfer along a hydrogen-bonded "wire"
09:15 – 10:00	Martina Havenith, Bochum Hydrogen Bonds: New Answers to old Questions
10:00 – 10:30	Coffee Break
Session 9	Chair: W.H. Eugen Schwarz, Siegen
10:30 – 11:15	Marius Lewerenz, Paris Vibrational Dynamics and Structure in Molecular and Ionic Clusters
11:15 – 12:00	Walter Thiel, Mülheim Ab Initio Vibration-Rotation Spectroscopy
12:00 – 14:00	Lunch Break
Session 10	Chair: Frédéric Merkt, ETH Zürich
14:00 – 14:45	Martin Suhm, Göttingen Vibrational Dynamics of Molecular Handshakes
14:45 – 15:30	Tomasz Wesolowski, Geneva Electron density partitioning as a route towards accurate multi-scale modeling of complex molecular systems and materials
15:30 – 16:00	Coffee Break

Wednesday, 1 October (continued)

Session 11	Chair: Kim Baldridge, Zürich
16:00 – 16:45	Joachim Sauer, Berlin Calculations on transition metal oxides - from gas phase clusters to solid catalysts
16:45 – 17:30	Claude Daul, Fribourg Modelling magnetic and spectroscopical properties of coordination compounds
17:30 – 18:00	Mitgliederversammlung: Arbeitsgemeinschaft für Theoretische Chemie
18:00 – 19:30	Dinner Break
	Mounting of Posters
19:30 – 22:00	Poster Session (ODD numbered)

Thursday, 2 October

Session 12	Chair: Jürgen Stohner, Winterthur
08:30 – 09:15	Jürgen Gauss, Mainz Rovibrational Spectroscopy and Quantum Chemistry
09:15 – 10:00	Markus Reiher, Erlangen Mode-Tracking: A new method for the calculation of pre-selected molecular vibrations
10:00 – 10:30	Coffee Break
Session 13	Chair: Ralph Jaquet, Siegen
10:30 – 11:15	Lorenz Cederbaum, Heidelberg Intermolecular decay and ultrafast energy transfer in clusters and weakly bound systems
11:15 – 12:00	William H. Miller, Berkeley Using the Initial Value Representation of Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations
12:00 – 14:00	Lunch Break
Session 14	Chair: Dominik Marx, Bochum
14:00 – 14:45	Nikos Doltsinis, Bochum Excited state tautomerism of the DNA base guanine
14:45 – 15:30	Michele Parrinello, Zürich/Lugano Calculation of free energy surfaces in classical and *ab-initio* molecular dynamics
15:30 – 15:35	Closing of the Meeting
	Departure

39th Symposium on Theoretical Chemistry
MOLECULAR SPECTROSCOPY AND DYNAMICS
28 September to 2 October 2003
Gwatt, Lake Thun, Switzerland

Organized by H.-P. Lüthi, M. Quack and J. Stohner

	Time	Sunday, 28 Sep	Monday, 29 Sep	Tuesday, 30 Sep	Wednesday, 1 Oct	Thursday, 2 Oct	Time
	8:30-9:15		Klopper	N.N. (Hellmann Lecture)	Leutwyler	Gauss	8:30-9:15
Morning	9:15-10:00		Luckhaus	Rizzo	Havenith	Reiher	9:15-10:00
Session	10:00-10:30		**Coffee Break**				10:00-10:30
8:30-12:00	10:30-11:15		Maier	Marquardt	Lewerenz	Cederbaum	10:30-11:15
	11:15-12:00	Arrival	Merkt	de Vivie-Riedle	Thiel	Miller	11:15-12:00
	12:00-14:00	and	**Lunch Break**				12:00-14:00
	14:00-14:45	Registration	Werner		Suhm	Doltsinis	14:00-14:45
Afternoon	14:45-15:30		Olsen		Wesolowski	Parrinello	14:45-15:30
Session	15:30-16:00	(from 3 pm)	**Coffee**	Excursion	**Coffee**		15:30-16:00
14:00-18:00	16:00-16:45		Frenking	or free	Sauer		16:00-16:45
	16:45-17:30		Hirao (PCCP Lecture)		Daul		16:45-17:30
	17:30-18:00				AGTC Meeting	Departure	17:30-18:00
	18:00-19:30	**Dinner**			**Dinner**		18:00-19:30
Evening	19:30-20:15	Troe	Poster Session	BBQ	Poster Session		19:30-20:15
Session	20:15-21:00	Jungen	(even numbered)	Dinner	(odd numbered)		20:15-21:00
19:30-22:00							

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