Sunday, July 11, 2011: Welcoming Reception 6:00 p.m. Stata (Building 32) 4th floor, R&D Common

MONDAY MORNING, JULY 11, 2011

8:30 AM Conference Welcome and Overview

Room 32-123

Session Chair: Nick Williams Room 32-123
8:40 AM Plenary Lecture: KINETIC STUDIES OF CHIRAL AMPLIFICATION IN AUTOCATALYTIC REACTIONS

Donna Blackmond, Scripps Research Institute

9:40 AM Poster Highlights 9:50 AM Refreshment Break

ORAL PRESENTATIONS - Session 1

Special Session: New Experimental Methods Chair: Robert Tranter Room 32-123	Catalysis 1 Chair: Preeti Aghalayam Room 32-141	Combustion Chemistry 1 Chair: O.O. Oluwole Room 32-144	Recombination, Roaming Chair: Ahren Jasper Room 32-155
10:20 AM PROBING KINETICS USING SYNCHROTRON RADIATION [#69] Musahid Ahmed	10:20 AM MECHANISMS AND RATES OF CATALYTIC REACTIONS FROM FIRST PRINCIPLES BASED THEORY [#253] William Goddard	10:20 AM A REDUCED CHEMICAL KINETICS MECHANISM FOR NOX EMISSION PREDICTION IN BIOMASS COMBUSTION [#106] Ehsan Houshfar	10:20 AM MOLECULAR SIZE DEPENDENT FALL-OFF RATE CONSTANTS FOR THE RECOMBINATION REACTIONS OF ALKYL RADICALS WITH O2 [#56] Akira Miyoshi
		10:45 AM A COMBINED MODELING AND EXPERIMENTAL STUDY OF THE COMBUSTION OF 1,3 BUTADIENE [#205] Marina Braun-Unkhoff	10:45 AM WHAT DO WE KNOW ABOUT THE ICONIC SYSTEM CH3 + CH3 ↔ C2H6? [#136] David Golden
11:05 AM ULTRAFAST TIME-RESOLVED X-RAY ABSORPTION SPECTROSCOPY: WATCHING ATOMS DANCE [#270] Christopher Milne	11:10 AM THE DIRECT EPOXIDATION OF PROPENE IN THE EXPLOSIVE REGIME IN A MICROREACTOR - A STUDY INTO THE REACTION KINETICS [#17] Alexander Niihuis	11:10 AM RADICAL CHEMISTRY IN THE THERMAL DECOMPOSITION OF ANISOLE: FORMATION OF BENZENE AND NAPHTHALENE [#50] Adam Scheer	11:10 AM THE KINETICS OF ROAMING RADICAL REACTIONS [#116] Stephen Klippenstein
	11:35 AM COMPUTATIONAL INVESTIGATION ON KINETICS OF SULFUR POISONING ON NICKEL CATALYSTS [#97] Teppei Oqura	11:35 AM ON THE COMBUSTION KINETICS OF PROPANOL [#189] Peter Lindstedt	
11:45 AM FREE RADICAL HETEROGENEOUS OXIDATION TRAJECTORIES [#114] Kevin Wilson Lunch Discussion to follow	12:00 PM THE DEVELOPMENT OF QUANTITATIVE INSIGHT INTO ALKENE METATHESIS CHEMISTRY [#120] Sara Kyne		12:00 PM COMPUTATIONAL STUDY ON THE RECOMBINATION REACTION BETWEEN BENZYL AND PROPARGYL RADICALS [#78] Akira Matsugi

12:25 PM

Break for Lunch (see map and restaurant info)

MONDAY AFTERNOON, JULY 11, 2011

ORAL PRESENTATIONS - Session 2

Rate Calculations	Rate Estimation	Low T	Catalysis 2	
Chair: Judit Zador	Chair: Elke Goos	Chair: Christa Fittschen	Chair: Guy Marin	
Room 32-123	Room 32-141	Room 32-144	Room 32-155	
1:50 PM MULTI-STRUCTURAL VARIATIONAL TRANSITION STATE THEORY [#265] Donald Truhlar	1:50 PM DETAILED CHEMICAL KINETIC MODELING OF JP-10 (EXO- TETRAHYDRODICYCLOPENTADIENE) HIGH TEMPERATURE OXIDATION [#51] Gregory Magoon	1:50 PM MASTER EQUATION CALCULATIONS FOR HYDROCARBON AND NITROGENOUS SPECIES REACTION RATE CONSTANTS AT LOW PRESSURES AND TEMPERATURES [#113] Gregory Smith	1:50 PM GAS PHASE KINETICS OF 1,3 BUTADIENE OXIDATION TO FURAN AND ISOBUTENE TO METHACROLEIN OVER BISMUTH- MOLYBDATE CATALYSTS [#255] Patrick Mills	
	2:15 PM ANALYSIS OF THE MAIN REACTION PATHWAYS ACTIVE DURING CYCLOPENTADIENE PYROLYSIS [#195] Carlo Cavallotti	2:15 PM REACTION INTERMEDIATES AT LOW TEMPERATURES: REACTION OF NITROGEN MONOXIDE WITH DIOXYGEN IN COLD GLASSY HYDROCARBONS [#159] Willem Koppenol	2:15 PM OXIDATION OF CIS-CYCLOOCTENE ON HETEROGENEOUS MN-TMTACN CATALYSTS [#224] Kathryn Bjorkman	
2:40 PM SEMI-CLASSICAL TRANSITION STATE THEORY APPLIED TO MULTIWELL CALCULATIONS ON THE OH+CO →H+CO2 REACTION [#216] Ralph Weston	2:40 PM TREE STRUCTURE FOR INTERMOLECULAR HYDROGEN ABSTRACTION IN HYDROCARBONS (C/H) AND GENERIC RATE CONSTANT RULES FOR ABSTRACTION BY VINYL RADICAL [#233] Sumathy Raman	2:40 PM EXPERIMENTAL INVESTIGATIONS OF RADICAL-MOLECULE REACTIONS USING LOW TEMPERATURE SUPERSONIC FLOWS [#254] Ian Sims	2:40 PM KINETICS OF NOX REMOVAL BY PEROXYDISULFATE ACTIVATED BY TEMPERATURE, TRANSITION METALS IONS AND ULTRASOUND [#200] Yusuf Adewuji	
3:05 PM NON-BORN-OPPENHEIMER MOLECULAR DYNAMICS AND TRANSITION STATE THEORY STUDY OF THE SPIN-FORBIDDEN H + HO2 → H2O + O(3P) REACTION [#177] Ahren Jasper	3:05 PM RATE CONSTANT ESTIMATION FOR LARGE CHEMICAL KINETIC MODELS AND APPLICATION TO BIOFUELS [#178] William Pitz		3:05 PM KINETIC STUDY OF COBALT(II) CATALYZED HYDROPEROXIDE ACTIVATION [#142] Ive Hermans	
3:30 PM THERMOCHEMISTRY, REACTION PATHS AND KINETICS ON THE ISOOCTANE RADICAL REACTIONS WITH 02 [#240] Suarwee Snitsiriwat		3:30 PM REACTIONS CH3 + OH, CH3 + CH3, AND OH + OH STUDIED OVER 1 - 100 BAR PRESSURE AND 298 - 715 K TEMPERATURE RANGES [#223] Lev Krasnoperov	3:30 PM METALLO-CATALYSTS FOR DESTRUCTION OF NEUTRAL ORGANOPHOSPHORUS PESTICIDES IN ALCOHOL. LARGE RATE ACCELERATIONS BROUGHT ON BY A MEDIUM EFFECT [#18] R. Stan Brown	
3:55 PM THEORETICAL STUDY ON THE MECHANISM AND KINETICS OF THE REACTION OF PHENYL RADICAL WITH PROPYLENE [#238] Vadim Kislov	3:55 PM COMPATIBILITY OF EXPERIMENTAL DATA FROM THERMAL AND CHEMICAL ACTIVATION [#168] Wing Tsang	3:55 PM PULSED LAVAL NOZZLE STUDIES OF THE KINETICS OF REACTIONS BETWEEN OH AND VARIOUS OXYGENATED VOCS AT VERY LOW TEMPERATURES [#141] Robin Shannon		
4:20 PM Adjourn to Poster Session (Sala de Puerto Rico, Building W-20 2nd floor)				

Adjourn to Poster Session (Sala de Puerto Rico, Building W-20 2nd floor)

TUESDAY MORNING, JULY 12, 2011

Session Chair: Ive Hermans Room 32-123

8:30 AM Plenary Lecture: HOMOLYTIC C-H BOND ACTIVATION: THE ROLE OF OXYGEN-CENTERED RADICALS AND MECHANISTIC ASPECTS Helmut Schwarz, Technische Universität Berlin

9:30 AM Poster Awards from Monday

9:45 AM Refreshment Break

ORAL PRESENTATIONS - Session 3

Butanol Chair: Mani Sarathy Room 32-123	De-Polymerization & Ring-Opening Pyrolysis Chair: Kevin Van Geem Room 32-141	Atoms & Ions Chair: Hans-Heinrich Carstensen Room 32-144	Reaction Kinetics Chair: Ravi Fernandes Room 32-155	
10:15 AM RATES OF H-ABSTRACTION FROM OXYGENATES; HOW DOES THESE DIFFER FROM HYDROCARBONS? [#62] Henry Curran	10:15 AM CHEMICAL ACTIVATION REACTIONS OF CYCLIC ALKANE, ETHER AND TRICYCLO DECANE RING-OPENED DIRADICALS WITH MOLECULAR OXYGEN: THERMOCHEMISTRY, REACTION PATHS AND KINETICS [#176] Itsaso Auzumendi-Murua	10:15 AM KINETICS OF ELEMENTARY STEPS IN THE REACTION OF ATOMIC BROMINE WITH 2,3-DIMETHYL-2- BUTENE UNDER ATMOSPHERIC CONDITIONS [#157] Patrick Laine	10:15 AM COMPOSITION BASED MODELING [#1] Steve Jaffe	
	10:40 AM MODELING THE THERMAL REARRANGEMENTS OF BICYCLIC MONOTERPENES [#161] Nick Vandewiele	10:40 AM THEORY OF ELECTROCHEMICAL KINETICS IN CONCENTRATED SOLUTIONS WITH APPLICATIONS TO LI-ION BATTERIES [#256] Martin Bazant	10:40 AM HIGH TEMPERATURE DISSOCIATION OF O- BENZYNE AND C6H5F [#232] Patrick Lynch	
11:05 AM COMBUSTION OF THE BUTANOL ISOMERS: REACTION PATHWAYS AT ELEVATED PRESSURES FROM LOW- TO-HIGH TEMPERATURES [#84] William Green	11:05 AM FIRST PRINCIPLES PREDICTION OF RATE COEFFICIENTS IN FREE- RADICAL POLYMERIZATION: SCOPE AND LIMITATIONS [#70] Michelle Coote	11:05 AM REACTIONS OF SULFUR ATOMS WITH H2 AND CS2: THE IMPORTANCE OF SPIN-FORBIDDEN PATHWAYS [#220] Paul Marshall	11:05 AM HIGH TEMPERATURE RATE CONSTANTS FOR D+C2H6 AND C3H8 [#64] Joe Michael	
11:30 AM MULTI-SPECIES MEASUREMENTS OF N-BUTANOL PYROLYSIS BEHIND REFLECTED SHOCK WAVES [#66] David Davidson		11:30 AM MONTE CARLO / RRKM / CLASSICAL TRAJECTORIES MODELING OF COLLISIONAL EXCITATION AND DISSOCIATION OF IONS IN MULTIPOLE COLLISION CELLS OF MASS SPECTROMETERS [#237] Vadim Knyazev	11:30 AM A SHOCK TUBE STUDY ON THE REACTION OF CYCLOHEXANE WITH H-ATOMS AND THE THERMAL DECOMPOSITION OF 1-HEXENE-6- YL RADICALS [#130] Sebastian Peukert	
11:55 AM DETAILED KINETIC MODELING OF PYROLYSIS AND COMBUSTION OF N- BUTANOL [#190] Alessio Frassoldati	11:55 AM RATES AND MECHANISMS OF THE THERMAL GAS-PHASE ISOMERIZATIONS AND DECOMPOSITIONS OF ETHYLCYCLOPROPANE AND 1,1- DIETHYLCYCLOPROPANE [#150] David Lewis	11:55 AM GAS PHASE ION CHEMISTRY: FROM ALPHA NUCLEOPHILES TO ALPHA CENTAURI [#180] Veronica Bierbaum	11:55 AM SHOCK TUBE STUDY ON THE REACTIONS NCN + H AND NCN + O [#110] Gernot Friedrichs	
12:20 PM RATE CONSTANTS FOR HYDROGEN- ABSTRACTION BY HO2• FROM n- BUTANOL [#61] Cheng-Wen Zhou	12:20 PM DETAILED KINETIC MODELING OF PYROLYSIS OF POLYISOPRENE [#251] Vinu Ravikrishnan		12:20 PM ISOTOPE EFFECT OF DEUTERATED METHOXY RADICALS (CH2DO) REACTING WITH O2 [#63] Hongyi Hu	
12:45 PM Butanol Lunch Discussion to follow				
	Afternoon free f	or Interactions or sightsoning		

Afternoon free for Interactions or sightseeing

5:00 p.m Poster Session Sala de Puerto Rico (Building W-20, Second floor)

7:00 p.m Conference Barbeque Sala de Puerto Rico

WEDNESDAY MORNING, JULY 13, 2011

Session Chair: David Golden

Room 32-123

8:30 AM Plenary Lecture: CHEMICAL KINETICS AND EARTH'S ATMOSPHERE: PAST, PRESENT, AND FUTURE -A.R. Ravishankara, NOAA - Boulder
9:30 AM Poster Awards from Tuesday
9:45 AM Refreshment Break

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	Special Session: Uncertainty Chair: Craig Taatjes Room 32-123	Computational Chemistry Chair: Jorge Aguilera Iparraguirre Room 32-141	Particle Systems & Interstellar Gas Chair: Richard West Room 32-144	Pyrolysis & Oxidation Chair: Linda Broadbelt Room 32-155	
	10:15 AM INTRODUCTION Craig Taatjes	10:15 AM PROPYL + 02: DEFINITIVE THEORY ON A PROTOTYPE OF HYDROCARBON OXIDATION [#266] Wesley Allen	10:15 AM OBSERVATIONS OF BROMINE EXPLOSIONS IN SMOG CHAMBER EXPERIMENTS ABOVE A MODEL SALT PAN [#219] Cornelius Zetzsch	10:15 AM GROUP-ADDITIVE KINETIC MODELING OF BIODIESEL PYROLYSIS: METHYLDECANOATE CASE STUDY [#36] Kevin Van Geem	
	10:25 AM METHODOLOGY AND INFRASTRUCTURE FOR PREDICTIVE MODELING [#165] Michael Frenklach		10:40 AM KINETIC MODEL FOR FLAME SYNTHESIS OF SILICA NANOPARTICLES FROM TEOS [#213] Markus Kraft	10:40 AM A KINETIC ANALYSIS OF THE SELECTIVE REMOVAL OF ETHYLENE AND PROPYLENE FROM SYNGAS VIA PARTIAL OXIDATION [#231] Stephanie Villano	
	11:05 AM THE ROLE OF SENSITIVITY ANALYSIS IN MODEL IMPROVEMENT [#122] Alison Tomlin	11:05 AM REACTION RATE RULES FOR HIGH AND LOW TEMPERATURE OXIDATION OF LARGE 2- METHYLALKANES [#148] Mani Sarathy	11:05 AM REDUCTION AND ANALYSIS OF DETAILED KINETICS FOR MODELING TIO2 NANOPARTICLE SYNTHESIS IN FLAME REACTORS [#24] Maulak Mehta	11:05 AM SHOCK TUBE MEASUREMENTS OF IGNITION DELAY TIMES AND OH AND H2O SPECIES TIME-HISTORIES IN 3-PENTANONE/02/AR MIXTURES [#65] David Davidson	
	11:45 AM DETERMINATION OF ARRHENIUS PARAMETERS BASED ON BOTH DIRECT AND INDIRECT MEASUREMENTS [#258] Tamas Turanyi Lunch Discussion to follow	11:30 AM ON UNDERSTANDING THE TEMPERATURE DEPENDENCE OF THE RATE CONSTANT FOR THE REACTION C2H5 + HBr → C2H6 + Br [#248] Paul Marshall & David Golden	11:30 AM REACTION KINETICS IN INTERSTELLAR CLOUDS OF GAS AND DUST: THE ROLES OF SURFACE AND GAS-PHASE CHEMISTRY [#267] Eric Herbst	11:30 AM FORMATION OF FUSED-RING AROMATIC COMPOUNDS FROM THE PYROLYTIC REACTIONS OF THE PHENYL RADICAL WITH ACETYLENE [#144] Andrea Comandini	
	12:25 PM	11:55 AM AN RRKM/ME ANALYSIS OF THE DECOMPOSITION KINETICS ACTIVE ON THE C7H6 POTENTIAL ENERGY SURFACE [#163] Daniela Polino		11:55 AM A QUANTITATIVE KINETIC ANALYSIS OF CO ELIMINATION FROM PHENOXY RADICALS [#218] Hans-Heinrich Carstensen	
١	12:25 PM Break for Lunch (see map and restaurant info)				

WEDNESDAY AFTERNOON, JULY 13, 2011

ORAL PRESENTATIONS - Session 5			
Atmospheric Chair: Theodore Dibble Room 32-123	Mechanisms (Condensed Phase) Chair: Carl Schiesser Room 32-141	Peroxyl Chair: Akira Miyoshi Room 32-144	Combustion Chemistry 2 Chair: Anthony Dean Room 32-155
1:50 PM TEMPERATURE DEPENDENT RATE COEFFICIENTS FOR OH + BUTANOL REACTIONS IN THE GAS PHASE [#49] Max McGillen	1:50 PM APPLICATION OF PSEUDO-FIRST- ORDER KINETICS TO FUNDAMENTAL ORGANIC REACTIONS [#10] Vernon Parker	1:50 PM DIRECT DYNAMICS VTST STUDIES OF UNIMOLECULAR REACTIONS OF N-PROPYL PEROXY RADICAL [#45] Feng Zhang	1:50 PM IMPROVED REACTION MECHANISM FOR COMBUSTION OF CORE COMPONENTS [#38] Chitral Naik
2:15 PM A THERMODYNAMIC AND KINETIC STUDY OF THE C6H5C•(=O) + O2 REACTION [#156] Joseph Bozzelli		2:15 PM PRESSURE DEPENDENT OH YIELDS IN ALKENE + HO2 REACTIONS: A THEORETICAL STUDY [#164] Judit Zador	2:15 PM ON THE CHEMICAL KINETICS OF AN UNSATURATED C7 ESTER: METHYL 3 HEXENOATE IGNITION AND SPECIATION STUDIES [#134] Scott Wagnon
2:40 PM THEORETICAL STUDY OF THE METHACROLEIN – OH REACTION IN AIR (#183) Gabriel da Silva	2:40 PM DEVELOPMENT AND APPLICATION OF A REAXFF REACTIVE FORCE FIELD FOR HYDROCARBON CRACKING ON A IRON EXCHANGED ZEOLITE [#171] Kaushik Joshi	2:40 PM MINOR PRODUCTS ANALYSIS DURING THE LOW TEMPARATURE OXIDATION OF ALKANES [#16] Frederique Battin-Leclerc	2:40 PM AN EXPERIMENTAL AND KINETIC MODELING STUDY OF N-PROPYLBENZENE OXIDATION AT TEMPERATURES OF 500–1000 K [#167] Saeed Jahangarian
3:05 PM ISOLATING INDIVIDUAL STEPS IN THE OXIDATION OF LARGE HYDROCARBONS: FORMATION OF SECONDARY ORGANIC AEROSOL VIA THE DIRECT PHOTOLYTIC GENERATION OF RADICAL SPECIES [#246] Jesse Kroll	3:05 PM STUDIES OF KINETICS AND MECHANISM OF REDOX REACTION BETWEEN GOLD(III) CHLORIDE COMPLEXES AND OXALIC ACID [#37] Krysztof Paclawski		3:05 PM UPDATED CHEMICAL REACTION MECHANISM FOR METHANE COMBUSTION AT HIGH PRESSURE [#194] Mayun Goswami
3:30 PM CHEMICAL FEEDBACKS ON THE ATMOSPHERIC LIFETIME OF NO AND NO2 RADICALS [#14] Ron Cohen	3:30 PM KINETICS OF COx FORMATION IN MC OXIDATION OF P-XYLENE [#99] Weizhen Sun	3:30 PM SYNCHROTRON PHOTOIONIZATION MEASUREMENTS OF BIOFUEL AUTOIGNITION CHEMISTRY: LOW- TEMPERATURE OXIDATION OF KETONES [#127] Subith Vasu	3:30 PM MODELING THE COMBUSTION OF HIGH MOLECULAR WEIGHT FUELS BY A FUNCTIONAL GROUP APPROACH [#235] Marco Mehl
	3:55 PM FIRST PRINCIPLE INVESTIGATIONS AND MOLECULAR DYNAMICS SIMULATIONS OF HETEROGENEOUS REACTION MECHANISM OF FORMALDEHYDE ON Fe(001) SURFACE AND COMPARISON WITH EXPERIMENTAL DATA [#245] Takahiro Yamada	3:55 PM LOW-TEMPERATURE PEROXY RADICAL ISOMERISATIONS IN ALKANE AUTOXIDATION AND ATMOSPHERIC CHEMISTRY [#260] Ive Hermans	3:55 PM KINETIC RESULTS FROM THE EXPERIMENTAL COMBUSTION OF CYCLOPENTADIENE DERIVED FROM A NEW C5 [#111] Robert Butler

THURSDAY, JULY 14, 2011

Session Chair: Anthony Dean Room 32-123

8:30 AM Plenary Lecture: A LASER FLASH PHOTOLYSIS STUDY OF CO2 REDUCTION: KINETICS LEADING TO THE DESIGN OF A RENEWABLE REDUCING AGENT - Barry Carpenter, Cardiff University 9:30 AM Poster Awards from Wednesday 9:45 AM Refreshment Break

ORAL PRESENTATIONS - Session 6

ORAL PRESENTATIONS - Session 0			
Special Session: Macromolecular Stress & Movement Chair: Nick Williams Room 32-123	R+O2 Chair: Jesse Kroll Room 32-141	Transients in Solution Chair: Francisco Sanchez Burgos Room 32-144	Nitrogen Chair: Gernot Friedrichs Room 32-155
10:15 AM KINETICS OF REACTIONS ACCELERATED BY MECHANICAL FORCE [#123] Stephen Craig	10:15 AM KINETICS AND OH YIELD MEASUREMENTS TO CONSTRAIN ENERGY BARRIERS IN THE CH3OCH2 + O2 REACTION [#132] Paul Seakins	10:15 AM DYNAMICS OF THE FORMATION OF SILVER DIMERS (AG2): SILVER NANOPARTICLES FROM CONCEPTION TO BIRTH [#271] Tito Scaiano	10:15 AM AB INITIO KINETICS AND MECHANISMS FOR SUBLIMATION OF AMMONIUM SALTS [#125] M.C. Lin
	10:40 AM ON PIMS STUDY OF METHYLPHENYL OXIDATION: ISOMER-SPECIFIC PRODUCT DETECTION [#244] Adam Trevitt		10:40 AM A DETAILED CHEMICAL KINETIC MECHANISM FOR THE OXIDATION OF MONOMETHYLHYDRAZINE [#170] Hongyan Sun
10:55 AM BARRIER COMPRESSION AND TUNNELING IN ENZYME CATALYSED REACTIONS [#21] Nigel Scrutton	11:05 AM INTERACTIONS OF THEORY, MODELING AND EXPERIMENT IN DETERMINING THE KINETICS AND MECHANISM OF ELEMENTARY REACTIONS [#242] Craig Taatjes	11:05 AM KINETICS OF THE LIQUID PHASE OXIDATION OF RENEWABLE OLEFINS [#139] Ive Hermans	11:05 AM VAPOR PHASE NITRATION OF ALKANE: UNDERSTANDING THE KINETICS OF KEY ELEMENTARY REACTIONS [#98] Debashis Chakraborty
11:40 AM CHOREOGRAPHING AN ENZYME'S DANCE - DYNAMICS DURING CATALYSIS [#272] Dorothee Kern		11:30 AM REACTION MECHANISMS OF CARBONATE RADICALS WITH AMINOCARBOXYLATE COMPLEXES IN AQUEOUS SOLUTIONS A PULSE RADIOLYSIS STUDY [#124] Israel Zilbermann	11:30 AM IMPROVED RATE CONSTANTS FOR NITROUS ACID DECOMPOSITION IN AQUEOUS SOLUTION AND KINETIC MODELLING OF NOX FORMATION FROM NITROSATING AGENTS [#68] Mark Rayson
Lunch Discussion to follow			
Conference Adjourns			