

Proposed program for the first ISSI meeting

Monday 7, January 2008 ----- Afternoon

14:00-14:30 Welcome and introduction to ISSI by *Vittorio Manno*

Session I: INTRODUCTION TO ASTROCHEMISTRY AND GAS-PHASE DATABASES

14:30-15:00 Introduction to Astrochemistry and its Uses in Astronomy
Ewine van Dishoeck

15:00- 15:30 Classes of Reactions used in Models: what is known and what is not known
Eric Herbst

15:30-16:00 Gas-Phase Networks and Models of Assorted Sources
Tom Millar

16:00-16:30 Coffee break

16:30-17:00 The Meudon PDR Code
Evelyne Roueff

17:00-18:00 GENERAL DISCUSSION:
completeness of models, problems including unusual reactions, astronomical uncertainties, heterogeneity, and time dependence

18:00 “Verre de l’amitié” offered by ISSI

Tuesday 8, January 2008

Session II: ESTIMATED UNCERTAINTIES IN RATE COEFFICIENTS AND HOW THEY ARE USED

9:00-9:30 Estimation of Rate Coefficient Uncertainties in Rate06
Andrew Markwick-Kemper

9:30-10:00 Uncertainty representation and propagation in chemical networks
Pascal Pernot

10:00-10:30 Coffee break

10:30-11:00 Abundance Uncertainties and Sensitivity Analyses in Cold and Hot Sources
Using osu.2008
Valentine Wakelam

- 11:00-11:30** Some Important Reactions
J.-C. Loison
- 11:30-12:30** GENERAL DISCUSSION:
which sensitivity methods are most useful?
How can one get useful uncertainties from uncritical databases such as NIST?

Session III: THEORY AND TEMPERATURE EXTRAPOLATION

- 14:30-15:00** Photoprocesses
Ewine van Dishoeck
- 15:00-15:30** Neutral-neutral & ion-molecule reactions: detailed theories
Juergen Troe
- 15:30-16:00** Low temperature extrapolations: methods of estimation
Ian Smith
- 16:00-16:30** Coffee Break
- 16:30-17:00** Ab initio potential surfaces and their uses
Dahbia Talbi
- 17:00-18:00** GENERAL DISCUSSION:
For what systems will theory be needed most? How accurate can ab initio +
dynamic methods be? What is the state of purely quantum mechanical
methods? Are modern statistical methods realistic?

Wednesday 9, January 2008

Session IV: GAS-PHASE EXPERIMENTS AND UNCERTAINTIES IN RATE
COEFFICIENTS

- 9:00-9:30** Ion-neutral reactions
Dieter Gerlich
- 9:30-10:00** Dissociative Recombination Reactions
Wolf Geppert
- 10:00-10:30** Coffee Break
- 10:30-11:00** Neutral-neutral reactions
Ian Smith

11:00-11:30 Critical Analysis of Conflicting Data: Previous Evaluations
Juergen Troe

11:30-12:30 GENERAL DISCUSSION:
Can experimental results be extrapolated to unstudied temperatures?
How do we learn about products in neutral-neutral reactions?
Why do different approaches to dissociative recombination reactions get different results?

Session V: SURFACE CHEMISTRY AND UNCERTAINTIES

14:30-15:00 H₂ formation in the laboratory: simple or complex?
Liv Hornekaer

15:00-15:30 The formation of polyatomic molecules in the laboratory
Harold Linnartz

15:30-16:00 Uncertainties in interstellar modeling: small particles, few reactive adsorbates
Eric Herbst

16:00-16:30 Coffee Break

16:30-17:00 Uncertainties in stochastic simulations
Herma Cuppen

Thursday 10, January 2008

9:00-10:00 GENERAL DISCUSSION:
Can reactions be studied in the laboratory on small particles?
Are there too many variables to allow modeling of interstellar surface chemistry?

Session VI: FUTURE GOALS

10:00-12:00 PANEL DISCUSSION (Valentine moderator):
what has been learned at the meeting? How do we go forward?

Participants

Nathalie Carrasco (Laboratoire de Chimie Physique, France)
Herma Cuppen (Leiden Observatory, The Netherlands)
Wolf Dietrich Geppert (Stockholm University, Sweden)
Prof. Dieter Gerlich (Technische Universitaet Chemnitz, Germany)
Eric Hébrard (Laboratoire Interuniversitaire des Systèmes Atmosphériques, France)
Prof. Eric Herbst (The Ohio State University, USA)
Liv Hornekaer (University of Aarhus, Denmark)
Harold Linnartz (Leiden Observatory, The Netherlands)
Jean-Christophe Loison (Institut des Sciences Moléculaires, France)
Andrew Markwick-Kemper (University of Manchester, UK)
Prof. Tom Millar (Queen's University Belfast, UK),
Pascal Pernot (Laboratoire de Chimie Physique, France)
Evelyne Roueff (LUTH, France)
Prof. Ian Smith (University Chemical Laboratory, UK),
Dahbia Talbi (Université de Montpellier, France)
Prof. Jürgen Troe (University of Göttingen, Germany)
Prof. Ewine van Dishoeck (Leiden Observatory, The Netherlands)
Valentine Wakelam (Laboratoire d'Astrophysique de Bordeaux, France)