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Atomic and Molecular Data for Plasma Modelling

Summary Report of First IAEA Research Co-ordination Meeting

IAEA, Vienna, Austria
26 – 28 September 2005

Prepared by
Denis Humbert

January 2006

IAEA NUCLEAR DATA SECTION, WAGRAMER STRASSE 5, A-1400 VIENNA

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Abstract

A brief description is given of the proceedings and conclusions of the first Research Coordination Meeting on “Atom and molecular data for plasma modelling”, held on 26-28 September 2005, at IAEA Headquarters in Vienna. Summaries are also given of the presentations made by the participants, along with the specific goals agreed for this Co-ordinated Research Project (CRP).

January 2006

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1. Introduction

The first Research Coordination Meeting (RCM) of the IAEA Co-ordinated Research Project (CRP) on “Atom and molecular data for plasma modelling” was held on 26-28 September 2005 at the IAEA Headquarters in Vienna. The objectives of the meeting were as follows:

1. summarize the current research activities of the participants,
2. formulate specific objectives for the CRP,
3. form a work plan among the participants to meet the specific objectives of the CRP.

Eleven CRP participants and two consultants attended the meeting: D. Herman (Czech Republic), K. Hassouni (France), U. Fantz, D. Reiter (Germany), M. Capitelli (Italy), M. Kimura, H. Tanaka (Japan), S. Matejcik (Slovak Republic), M. Larsson (Sweden), J. Tennyson (United Kingdom), B. J. Braams (USA) and J. Hogan (USA). Both B. McLaughlin (United Kingdom, CRP participant) and R. K. Janev (Macedonia, consultant) were unable to attend. The Agency was represented by A. L. Nichols, R. E. H. Clark and D. Humbert. The list of participants is attached as Appendix 1.

2. Overview

Attendees at the meeting were welcomed by A. Nichols (Head, Nuclear Data Section). The proposed Agenda had been divided into six sessions, and was adopted without any changes (Appendix 2). The first four sessions were devoted to reports from the participants of their latest research activities. Brief summaries of the presentations are reported below, while full presentations are available on the Web site of the A+M Data Unit (<http://www-amsdis.iaea.org>). The fifth session included discussions and a formulation of specific objectives for the CRP, matching these objectives with the capabilities of individual participants. The last session was devoted to debating and agreeing the conclusions of the meeting. A document was also prepared that identified the specific tasks to be performed by each participant in order to fulfil the overall objectives of the CRP (see Section 4).

3. Summaries of Research

3.1. Session 1

Chaired by U. Fantz, the first session focused on experimental research, and included presentations from M. Larsson, D. Herman and S. Matejcik.

M. Larsson: Dissociative recombination of hydrocarbon ions

Dissociative recombination of hydrocarbon ions is expected to take place in the divertor region of a thermonuclear fusion reactor. The process has been studied at the CRYRING ion storage ring over the previous three years, particularly product branching ratios and the development and expansion of the database. A review of this work was given, and a programme for the CRP was outlined.

Zdenek Herman: Energy transfer, dissociation and chemical reactions in collisions of slow polyatomic ions with surfaces

Surface-induced dissociation and reactions in interactions of polyatomic ions with different surfaces (surfaces with self-assembled monolayers, carbon surfaces, hydrocarbon-covered metal surfaces) were studied using the scattering method. The projectile ions were ethanol

and benzene molecular ions, and small $C_1 - C_3$ hydrocarbon ions, CH_n^+ ($n = 3-5$), $C_2H_n^+$ ($n = 2-5$), $C_3H_n^+$ ($n = 3-8$), and their D- and ^{13}C -labelled variants.

A mass-selected beam of projectile ions (incident energy in the range of 5-50 eV) of narrow angular (1.5°) and energy (about 200 meV) distribution is directed under a pre-selected angle to the surface (at room temperature or heated to about 1000K). Ions scattered off the surface are subjected to energy and angular analysis, and are recorded by means of a mass spectrometer.

Energy transfer and partitioning of the incident projectile energy into internal excitation of the projectile, translational energy of products, and energy absorbed by the surface was determined from mass spectra, translational energy and angular distributions of the product ions upon impact of ethanol molecular ions [1-3]. Dissociation of the polyatomic projectile occurred after the interaction with the surface. The distribution function for the translational-to-internal energy transfer peaked at 17% of the incident energy for the perfluoro-hydrocarbon SAM [3], and at about 6% for the other surfaces investigated. The fraction of energy remaining as product translational energy decreased with increasing incident angle (with respect to the surface) and the fraction of energy absorbed by the surface increased correspondingly.

The ion survival probability was about a factor of 30-50 larger for closed-shell ions than for open-shell radical cations (e.g., 12% for CD_5^+ vs. 0.3% for CH_4^+ , $\Phi_N = 60^\circ$), and depended strongly on the incident angle [1, 4].

The main chemical reaction with surfaces covered by a hydrocarbon layer was H-atom transfer to the projectile radical cation [1-4]. Formation of C_2 (mainly $C_2H_3^+$ in reactions of C_1 hydrocarbon ions) and C_3 hydrocarbon ions (mainly $C_3H_3^+$ in reactions of C_2 hydrocarbon ions) was observed for small hydrocarbon ion projectiles in reaction with the surface terminal CH_3 - group [4].

The initial internal energy content of the projectile ion seems to be fully preserved in the projectile during the ion-surface collision and available for further dissociation of the surface-excited projectile ion [5].

- [1] J. Kubišta, Z. Dolejšek, Z. Herman, European Mass Spectrom. **4** (1998) 311-320.
- [2] J. Žabka, Z. Dolejšek, J. Roithová, V. Grill, T. D. Märk, Z. Herman, Int. J. Mass Spectrom. **213** (2002) 145-156.
- [3] J. Žabka, Z. Dolejšek, Z. Herman, J. Phys. Chem. **A106** (2002) 10861-10869.
- [4] J. Roithová, J. Žabka, Z. Dolejšek, Z. Herman, J. Phys. Chem. **B106** (2002) 8293-8301.
- [5] A. Qayyum, T. Tepnual, C. Mair, S. Matt-Leubner, P. Scheier, Z. Herman, T. D. Märk, Chem. Phys. Lett. **376** (2003) 539-547.

Stefan Matejčík: Formation of positive ions by electron impact - temperatures effects

The threshold behaviour of the cross section for cations formed via electron impact ionization to methane (CH_4 , CH_3D and CD_4), ethane (C_2H_6) and propane (C_3H_8) has been studied in a crossed electron/neutral beams apparatus with mass spectroscopic analysis of the ions. The appearance energies (AEs) of the ions formed via electron impact ionization of these molecules were determined at room and at elevated temperature (about 700K). At elevated gas temperatures a decrease of the appearance energies has been observed for all molecules (red shift). The red shift appears to depend on the size and isotopic composition of the

molecules. These results indicate that at very high gas temperatures the cross sections for electron impact ionization in the threshold region may substantially differ from those at low temperature. Additionally, differences in the appearance energies due to isotopic substitution have been observed for CH₄, CH₃D and CD₄ molecules.

3.2. Session 2

This session was chaired by M. Kimura, emphasized data users, and included presentations from K. Tanaka, J. T. Hogan and D. Reiter.

Hiroshi Tanaka: Electron collision data for C-H compound molecules for fusion plasma modelling

An overview was given of the possible contribution of the Department of Physics of Sophia University to the CRP, including measurements of low-energy electron scattering on hydrocarbons and data compilation from the available literature. Current activities were described within the department on data compilation, data measurements and calculation, including various collaborations.

A joint project between Australia, Japan and South Korea on “scattered electron collision data” has been underway since 1990 - data are being collected to complete already existing fusion-related databases. Measurements are undertaken in different facilities: Spring-8, RIKEN, Sophia. This experimental work involves a long list of molecules including hydrocarbons:

- Electron Energy-Loss Spectroscopy (EELS): elastic scattering differential cross sections (DCS), resonant phenomena in vibrational excitation, electronic excitation, and generalized oscillator strength (GOS);
- Quadrupole Mass Spectrometry (QPMS): non-radiative dissociation, threshold ionization energy, and dissociative attachment;
- Low Energy Electron Diffraction (LEED): surface and phase transition.

The Department of Physics at Sophia also has some computing facilities on which calculations of low-temperature RF plasmas can be carried out.

John Hogan: Need for improved hydrocarbon data in the modelling of the generation and transport of intrinsic impurities and their influence on tritium (deuterium) retention

The way in which existing cross sections and rate coefficients for hydrides and isotopes are used in plasma edge modelling codes can be illustrated through model comparisons with data for core and divertor ELM dynamics (DIII-D), ELM heat flux mitigation (JET), evaluation of co-deposition as a possible long-term retention mechanism (Tore Supra), the relationship between particle-induced desorption and chemical erosion in retention (JET), and the study of simpler experiments that might be used to validate improved rate calculations. Many seemingly disparate and complex processes are closely linked, and this situation provides the motivation for the creation of a systematic atomic and molecular database.

Detlev Reiter: Atomic and molecular data issues for ITER, and status of databases for the EIRENE code

D. Reiter discussed atomic and molecular data issues for magnetic confinement fusion reactors, and focused on the ITER project. A plasma detached regime seems more appropriate for ITER, protecting the chamber from the flux of particles with a reactive plasma. Remaining major issues are the tritium retention and removal from the chamber, and

a better understanding of the plasma behaviour in the divertor region. The Monte-Carlo neutral gas transport code EIRENE, connected with the plasma fluid dynamics code B2 is used for the design of the ITER divertor. The comparison of the A+M and surface interaction databases coupled with the B2-EIRENE demonstrates a need for more accurate data, especially at low energies and for hydrocarbons.

3.3. Session 3

The next two sessions focused on data producers. Session 3 was chaired by J. Tennyson, and included presentations by K. Hassouni, M. Kimura and B.J. Braams.

Khaled Hassouni: Modelling of hydrocarbon plasmas used for carbon material processing - current status with respect to collisional data

These studies deal with specific aspects of the modelling of H_2 , H_2/CH_4 and $Ar/H_2/CH_4$ microwave plasmas used for diamond films deposition, with significant emphasis placed on the problems related to collisional data.

The first part of the presentation dealt with kinetics modelling and the development of a collisional radiative model for a pure H_2 plasma. Investigations of the effect of excited states on the overall dissociation and ionization kinetics performed with these models were also presented. This model can be reduced to obtain simple and accurate chemical models that may be used in transport codes and in the modelling of the more complex H_2/CH_4 plasmas.

Mineo Kimura: Charge transfer and fragmentation in ion-molecules collisions below keV energies

An investigation has been made of charge transfer processes in ion-molecules collisions for various hydrocarbons and non-hydrocarbon molecules below keV energies. New findings include a strong temperature effect, and significant isotope and isomer effects, as well as a conspicuous steric effect, all of which have not been observed previously. These findings demand new analysis of previous experimental results and interpretation of their physics. The majority of molecular ions formed after charge transfer are known to be unstable and undergo fragmentation. Studies have also been carried out on the fragmentation mechanism and the corresponding production of fragmented species.

Other work addresses the one-dimensional transport modelling of H_2 and H_2/CH_4 plasmas. The main phenomena and processes that govern the spatial distribution of plasma temperatures and active species were debated. Discussions also focused on the key processes that result in the formation of sooty $Ar/CH_4/H_2$ discharges from some reaction mechanisms.

Results were analyzed to determine the main collisional processes that govern the investigated discharge. The main collisional data necessary for accurate prediction of the discharge characteristics and process simulation were discussed. Furthermore, the sensitivity of the results to the value of some collision cross sections were noted, and general guidance was given on the different collisional data for which accurate measurements or theoretical prediction are still needed for the modelling of moderate pressure hydrocarbon discharges.

Bastiaan J. Braams: Construction of global potential energy surfaces for small molecules, with a view to breakdown of methane and ethene in a plasma

Over the previous two years, the Bowman group at Emory University has constructed full-dimensional potential energy surfaces for a variety of molecular systems, including H_5^+ , CH_5 , CH_5^+ , $H_3O_2^-$, H_4O_2 , $H_5O_2^+$, C_2H_2O , C_3H_3O , CH_2O , C_3H_2 and $HOONO$ (for example, Ref.

[1]). A dipole moment surface was constructed for some of these systems. These surfaces were obtained by global least-squares fitting to the results of typically several times 10^4 high level *ab initio* calculations. The property of invariance under permutations of like nuclei was built into the least-squares fitting procedure, and the MAGMA computer algebra system was used to help generate the codes. A cluster expansion (many-body expansion), with up to five-body or at most six-body terms, caters for dissociation and reaction processes, and can also be extended to larger systems. The fitted potential and gradient are evaluated on a millisecond timescale, so that molecular dynamics or quantum Monte-Carlo calculations can be carried out to *ab initio* accuracy without the cost that is normally associated with *ab initio* MD, or even with a Car-Parrinello treatment. The fitted surfaces have also been used for MULTIMODE calculations of a vibrational spectrum. These methods were discussed, along with application to reactions of methane and ethane, and their breakdown products with H, H⁺, H₂ and H₂⁺ in the plasma.

- [1] X. Huang, B. J. Braams, and J. M. Bowman, *Ab initio* potential energy and dipole moment surfaces for H₃O₂⁺, J. Chem. Phys. **122** (2005) 044308.

3.4. Session 4

This session was chaired by B. J. Braams, and included presentations by J. Tennyson, M. Capitelli and U. Fantz.

Jonathan Tennyson: R-matrix calculations of electron-molecule collisions at low and intermediate energies

The R-matrix method is now well-established as a reliable and flexible procedure for treating electron collision problems. UK molecular R-matrix codes in particular have been applied to an increasing variety of electron molecule collision problems. Recent calculations on low-energy electron collisions with water have exhibited outstandingly good agreement with published measurements of differential and momentum transfer cross sections. However, the calculated elastic cross sections differ significantly from those inferred from experiment, suggesting that the published data still do not correctly measure the strong forward peak for this process. New calculations have been performed on the 13-atom organic ring molecule tetrahydrofuran with special attention paid to the low-lying resonances in this system, and a new molecular R-matrix with a pseudo-states (MRMPS) procedure has been developed that allows the correct *ab initio* treatment of electron collision processes, including ionisation above the molecular ionisation threshold. Initial studies on benchmark systems suggest that this method works well. Also, as part of the CPR, Tennyson *et al.* have initiated a study of electron collisions with the carbon dimer.

Mario Capitelli: Dynamics, kinetics and modelling of molecular and atomic plasmas – state-to-state approach

Modelling of molecular and atomic plasmas requires a large amount of information about the elementary processes acting in the plasma. This information increases exponentially when the description includes the non-equilibrium distributions existing in the plasma, and therefore the state-to-state approach becomes necessary in order to understand the complex phenomenology occurring in the plasma. This situation arises in the case of H₂/D₂ plasmas for negative ion sources, as well as for N₂ and O₂ plasmas occurring under many circumstances.

Ursel Fantz: Compilation and extension of a database for systematic studies on diatomic molecules

Available tools for calculating basic molecular data and particle densities relevant for plasma edge modelling were briefly introduced. The TraDiMo code is capable of calculating eigenvalues, Franck-Condon factors, vibrationally-resolved transition probabilities, effective transition probabilities and branching ratios for diatomic molecules on the basis of potential curves and dipole transition moments. Yacora is a flexible code for the calculation of particle densities in vibrationally-resolved excited states (collisional radiative modelling), or reaction chains (dissociation model). Results were given for hydrogen and associated isotopomers for which a complete database has already been made available. The application of these tools to CH, BH, BeH and their hydrogen isotopes as well as C₂ was discussed. These studies require the compilation and evaluation of data, i.e. potential curves, dipole transition moments, rate coefficients or cross sections. Based on the Born approximation, the IPProg code calculates electron impact excitation rate coefficients, and has been applied to diatomic molecules. Results were compared with the available data. The possibility of using Yacora for dissociation modelling of hydrocarbons and hydrogen based on different available databases was also discussed, and the importance for the identification of relevant heavy particle collisions was noted.

4. Objectives and Work Plan

4.1. Introductory remarks

D. Reiter chaired a session in which all relevant on-going research was summarised, and a list of data requirements and a work plan for this CRP were formulated. J. T. Hogan undertook the task of rapporteur, and participants commented on and suggested changes as the discussions unfolded.

Bob Clark summarized the status of the current and foreseen CRPs of the A+M Data Unit of the IAEA, in order to complement these efforts and minimize possible duplication of effort. The list of A+M CRPs is as follows:

1. Data for molecular processes in edge plasmas, 2001-2005 (*ending*).
2. Tritium inventory in fusion machine, 2002-2006.
3. Atomic and molecular data for plasma modelling (*this CRP*).
4. Atomic data for high Z element impurities in fusion reactors, 2005-2008.
5. Data for surface composition dynamics relevant to erosion processes, 2006 (*planned*).

More information on these CRPs can be found on the A+M Data Unit Web site (<http://ww-amdis.iaea.org>).

4.2. Specific research objectives and tasks

The CRP will focus on gathering and generating new data relevant to modelling the edge region of plasmas within nuclear fusion energy devices. The work plan is divided into two topics: one related to plasma surface interactions, and the other focused on volume processes.

Surface processes

Include low-energy D and chemical reactions for $C \rightarrow C_3$ hydrocarbons for energies from 1 to 10 eV (consider neutrals as well as ions) and evaluate present database. Also investigate other surfaces: Be and W, and compare ion survival from C/Be/W [Zdenek].

Evaluate the Alman/Ruzic/Brooks surface database in fusion plasma modelling “A hydrocarbon reaction model for low temperature hydrogen plasmas and an application to the Joint European Torus”, D. Alman, D. Ruzic, J. Brooks, *Physics of Plasmas* **7** (2000) 1421 [Hogan, Reiter].

Determine experimental signatures of surface productions of molecules such as C_2H_2 and other ITER relevant molecules, as well as diamond-like carbon (DLC). Mass spectrometry. Evaluate present database [Hassouni].

Most basic hydride - study recombination of atomic H/D onto graphite to understand formation of vibrational excited molecules [Capitelli].

Volume processes

Scheme:

QC \rightarrow
scattering theory/experiment \rightarrow
experimental validation (spectroscopy, fusion experiments) \rightarrow
relevant fusion applications (ITER)

Calculate ground state potential energy surfaces for hydrocarbons to C_2H_6 [Braams].

Evaluate cross-section reaction rates (vibrational and rotationally-resolved) for reactions proceeding on the ground state surface; evaluate the relevance of ground state restriction to edge plasma processes. Provide ionization potentials, thresholds, ro-vibrational cross sections and spectroscopic data for reactions [Braams].

Complete database of e-collision cross sections for vibrational excited molecules (D_2 , DT, T_2), and continue work on atom-diatom, electron-molecule collisions [Capitelli].

Calculate electronic structure, binding energy, volatility affinities and ionization energies for $Be_{1,2}$, hydrides and H_2 reactions with Be_n clusters [Matejcik].

Calculate excited state molecular structure up to C_4H_8 .

Evaluate CO sticking on metallic substrate surfaces (Ag) [Kimura].

Determine charge-transfer cross sections in collisions of H^+ , He^{2+} and C^{q+} ions with hydrocarbons and other fusion-relevant molecules systematically below 50 keV/u [Kimura].

Determine fragmented species from impurity molecules after charge transfer and ionization, and their energy distributions [Kimura].

Evaluate theoretical cross sections (R-matrix) on total, elastic and inelastic electronic excitation (energy 1-10 eV) of the diatomic molecules BeH, BeD, CD and C_2 . Then extend to the polyatomic systems, BeH_y and isotopomers, and hydrocarbon molecules (CH, C_2H_2 and C_2) [Tennyson, McLaughlin].

Benchmark C_2H_2 rates, electron collision cross sections.

Elastic, vibrational and electronic excitation (break-up) [Tennyson, McLaughlin, Tanaka].

Ionization data for C_2H_2 [Braams, used as input by Hassouni].

Closed shell hydrocarbon molecules:

- 1) provide missing but necessary experimental data - cross sections for the excited neutral molecular species and the emissive radical production from C-H compound molecules by low-energy electron impact;
- 2) unification of database for the modelling at Jülich, and updating of the database [Tanaka et al].

Merged and completed databases to be available both from FZ-J and IAEA NDS A+M Unit [Reiter, Janev, Clark].

C_3H_x ionic systems - recombination, and dissociation excitation.

Cross sections as well as rates. Evaluate relevance of BeH^+ , BeH_2^+ [Larsson].

Measure ionization - cross sections in threshold region to 10 eV above, for CH_4 , C_2H_6 , C_3H_8 and fragments. Propane cross section at elevated T of 700K [Matejcik, Hassouni].

CR modelling, data from Bari for H_2 (D_2). Differences in excitation for isotopes? Validate for HD in ECR discharges.

CR modelling for C_2/CH molecules - FC factors, systematic transition probabilities, and eventually BeH/BH for diagnostic applications.

CR/dissociation modelling to determine PECs for CH , C_2 , H_2 to test available databases, and generate information about recombination processes. ECR plasmas + AUG/DIII-D comparisons.

See how heavy-particle collisions influence dissociation modelling, and determine relevance to divertor plasmas [Fantz].

Extend model used previously to study DLC to lower pressure (few Pa) with PIC for C_2H_2 and CH_4 to deduce main species, plasma and surface chemistry from experiments - e-impact vs CX [Hassouni].

Apply CR model to H_2-H system in order to evaluate the validity of this approach through collaboration with Augsburg/AUG [Hassouni, Fantz, Capitelli].

Line shapes (CH , C_2 , C) to give information on kinetics of break-up [Fantz].

Integrated modelling for tokamaks, stellarators and ITER. Evaluation of the impact of new data on plasma observables, especially through spectroscopy. Assess and report differences in database predictions for hydrocarbon break-up chain-integrated models (for example, J-R vs E-L, A-R). Direct application to JET and ITER divertor modelling. Assess sensitivity to break-up kinetic energies, and evaluate effects on line shapes (CH , C_2 , C) [Hogan, Reiter].

5. Conclusions

The CRP on “Atomic and molecular data for plasma modelling” will focus on gathering and generating new data relevant to the edge region of plasmas in nuclear fusion energy devices. This first RCM revealed a good match between the expertise of the participants and the identified needs in this area. A detailed work plan has been established to cover the timescale leading to the next CRP meeting (to be held in spring 2007), at which point an evaluation will be made of the status of the work along with an assessment of the additional data needs. Mechanisms have been established for producing the required data, and for incorporating the newly generated data into existing databases, for merging and completing databases in this area, for validating the data in plasmas, and for using these data in fusion plasma modelling.

**First IAEA Research Co-ordination Meeting on
Atomic and Molecular Data for Plasma Modelling**

26-28 September 2005, IAEA Headquarters, Vienna, Austria

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**First IAEA Research Co-ordination Meeting on
Atomic and Molecular Data for Plasma Modelling**

26-28 September 2005, IAEA Headquarters, Vienna, Austria

Agenda

Monday 26 September

Meeting Room: A-07-42

09:30-10:00 Opening, Adoption of Agenda, A. Nichols, R.E.H. Clark, D. Humbert

Session 1: Scientific Reports

Chairman: U. Fantz

- | | | |
|---------------|---------------------|--|
| 10:00 - 10:45 | M. Larsson | Dissociative recombination of hydrocarbon ions |
| 10:45 - 11:15 | <i>Coffee Break</i> | |
| 11:15 - 12:00 | Z. Herman | Energy transfer, dissociation and chemical reactions in collisions of slow polyatomic ions with surfaces |
| 12:00 - 12:45 | S. Matejcik | Formation of positive ions by electron impact: Temperatures effects |
| 12:45 - 14:00 | <i>Lunch</i> | |

Session 2: Scientific Reports

Chairman: M. Kimura

- | | | |
|---------------|---------------------|---|
| 14:00 - 14:45 | H. Tanaka | Data needs for electron interaction with plasma processing and fusion plasma gases |
| 14:45 - 15:15 | <i>Coffee Break</i> | |
| 15:15 - 16:00 | J.T. Hogan | Need for improved hydrocarbon data in modeling of the generation and transport of intrinsic impurities and their influence on tritium (deuterium) retention |
| 16:00 - 16:45 | D. Reiter | Atomic and molecular data issues for ITER, and status of databases for the EIRENE code |

Tuesday 27 September

Session 3: Scientific Reports

Chairman: J. Tennyson

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|---------------|-------------|--|
| 09:30 - 10:15 | K. Hassouni | Modeling of hydrocarbon plasmas used for carbon material processing. Current status with respect to collisional data |
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10:15 - 11:00	M. Kimura	Charge transfer and fragmentation in ion-molecules collisions below keV energies
11:00 - 11:30	<i>Coffee Break</i>	
11:30 - 12:15	B.J. Braams	Construction of global potential energy surfaces for small molecules, with a view to breakdown of methane and ethene in plasma
12:15 - 14:00	<i>Lunch</i>	

Session 4: Scientific Reports

Chairman: B.J. Braams

14:00 - 14:45	J. Tennyson	R-matrix calculations of electron-molecule collisions at low and intermediate energies
14:45 - 15:15	<i>Coffee Break</i>	
15:15 - 16:00	M. Capitelli	Dynamics, kinetics and modeling of molecular and atomic plasmas: the state to state approach
16:00 - 16:45	U. Fantz	Compilation and extension of a database for systematic studies on diatomic molecules

Wednesday 28 September

Session 5: CRP work plan

Chairman: D. Reiter

09:00 - 10:45	All	Discussion of reports and work plan for the next 3 years
10:45 - 11:15	<i>Coffee Break</i>	
11:15 - 12:30	All	<i>(continued)</i>
12:30 - 14:00	<i>Lunch</i>	

Session 6: Formulation of meeting conclusions

Chairman: M. Capitelli

14:00 - 17:00	All	Formulation of meeting conclusions
17:00 -		<i>Adjournment of Meeting</i>

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