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Atomic and Molecular Data for Plasma Modelling

Summary Report of the final Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

17 – 19 November 2008

Prepared by

Denis Humbert
International Atomic Energy Agency, Vienna, Austria

February 2009

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Abstract

The final Research Coordination Meeting on "Atom and Molecular Data for Plasma Modelling" of the Coordinated Research Project (CRP) was held on 17-19 November 2008, at IAEA Headquarters in Vienna. Participants summarized the results obtained in the course of the CRP, and the impact of the data on modelling, especially for the plasma edge and divertor regions. Data needs still exist, and the specialists hoped that further research on these processes will be supported in the future. The discussions, conclusions and recommendations of the RCM are described in this report.

February 2009

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Introduction

The final Research Coordination Meeting (RCM) of the IAEA Coordinated Research Project (CRP) on "Atom and Molecular Data for Plasma Modelling" was held on 17-19 November 2008 at the IAEA Headquarters in Vienna. This meeting was saddened by the news that Mineo Kimura, representative of Kiushu University, passed away in February 2008. Kimura had been collaborating for many years with the Atomic and Molecular Data Unit, as a participant in two CRPs and consultant within many CMs. Hirohito Tanaka gave a short presentation in his memory. The existing CRP and the AM Data Unit will miss his high level of competence in atomic and molecular physics, and his cheerful personality.

The objectives of the meeting were as follows:

1. review the progress made by participants with respect to the work plan,
2. review the achievements made on the specific objectives of the CRP,
3. identify needs for further research.

12 CRP participants attending the meeting: Z. Herman (Czech Republic), U. Fantz, D. Reiter (Germany), M. Capitelli (Italy), H. Tanaka (Japan), S. Matejcik (Slovak Republic), M. Larsson (Sweden), J. Tennyson (United Kingdom), B. J. Braams (USA), D. Schultz (USA), B. McLaughlin (United Kingdom) and R. K. Janev (Macedonia). K. Hassouni (France) had proffered his apologies for absence. M. Bannister from ORNL (USA) attended the meeting as observer. The Agency was represented by A. L. Nichols, R. E. H. Clark and D. Humbert. The list of participants is attached as Appendix 1.

Overview

Attendees at the meeting were welcomed by A. Nichols (Head, Nuclear Data Section). He commented on the strong support of the Agency, the Division and the Section to fusion activities. Fusion is foreseen as a future long-term energy supplier, and the need for high quality data for fusion reactor was noted. Following the introduction the proposed Agenda was reviewed and adopted without change (Appendix 2). The two first days were devoted to reports from the participants on their latest research activities related to the CRP, each participant giving forty-five minute talks, including questions. Brief summaries are reported below, while full presentations are available on the Web site of the A+M Data Unit (http://www-amdis.iaea.org). Much discussion resulted from the presentations, and areas with need for further research were noted. Late Tuesday afternoon and Wednesday included detailed discussions and preparation of an agreed summary of work achieved during the CRP. Further data needs for plasma modelling were identified.

Presentations of Work Performed

Over the course of the two first days, each participant gave a summary presentation of results achieved since the second RCM. Each participant gave a forty-five minute presentation including questions. These presentations are available at
http://www-amdis.iaea.org/CRP/Plas_Mod/RCM3/presentations/

Zdenek Herman: "Interaction of Slow Ions with Surfaces: **Ion Survival Probability on Carbon, Tungsten and Beryllium Surfaces (Room Temperature and Heated)"**

Zdenek Herman reviewed earlier and new data on absolute survival probabilities of hydrocarbon ions C, C_2, C_3, and some other ions, obtained at J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Prague. Measurements were performed for room temperature and heated (600ºC) surfaces of carbon (HOPG), tungsten and beryllium. The correlation of the results

with the ionization energy of the different studied projectile ions was discussed. This correlation may help to estimate survival probabilities of other ions.

Dave Schultz and Mark Bannister: "Electron - hydrocarbon molecular ion reactions"

Mark Bannister and Dave Schultz presented a survey of the electron-hydrocarbon molecular ion reactions that have been measured at the Oak Ridge National Laboratory Multicharged and Molecular Ion Research Facility (MIRF), as well as considering those reactions that will be measured in the near future. These data are intended to provide a benchmark for key collision systems in order to test and refine the existing database of electron-hydrocarbon reactions of relevance to ITER edge and divertor modelling. They also displayed comparisons of the data measured at MIRF with the recommended values contained in the Julich reports and HYDKIN. Finally, preliminary results of a novel molecular dynamics-energy deposition model were described. The aim of this model is to provide results for a wide range of electron-hydrocarbon reactions with a single readily tractable approach since the full quantum mechanical treatment must be especially tailored for each system and requires very significant computational and human effort.

Stefan Matejcik: "Electron Impact Ionization Studies of Small Hydrocarbons and Beryllium Compounds"

Stefan Matejcik presented the latest results obtained at the Department of Plasmaphysics, Comenius University, Bratislava, Slovakia.

The partial cross sections of Electron Impact Ionization (EII) of the C_3H_8, C_2D_6 and CHD_3 molecules have been measured in the electron energy range from threshold up to 150 eV. The influence of the gas temperature on the cross sections has been studied. Additionally, the appearance energy of the ions formed by EII to $C_3H_6D_2$ has been measured at low and high temperatures.

Theoretical structure and energetics and excited states of the beryllium hydrates have been studied and the cross sections for EII to various beryllium hydrates have been calculated.

Bastian J. Braams: "Potential energy surfaces and applications for hydrocarbons"

Bastian Braams reviewed work done with the group of Joel M. Bowman at Emory University on the construction of potential energy surfaces for small molecules, especially hydrocarbons, and the use of these surfaces for spectroscopy and reaction dynamics. Hydrocarbon applications include the study of the ro-vibrational spectrum of CH_4, CH_5^+, C_2H_3, $C_2H_3^+$ and $C_2H_5^+$, reaction dynamics of C^+ - C_2H_2 and dissociative recombination of CH_5^+. The CH_4 study opens up a new field of application by demonstrating this approach for obtaining a comprehensive set of emission and absorption coefficients for millions of lines for use in radiation transport modelling.

Limitations of the present work were indicated. Issues of electronic excited states and the associated surface crossings and conical intersections in the reaction dynamics studies are not yet properly covered. These issues must be addressed as almost every ion-neutral interaction involves multiple electronic surfaces to account for charge transfer.

M. Larsson: "Calculations on BeH^+"

Dissociative recombination of BeH^+ had not been studied earlier by either experimental or theoretical methods. Mats Larsson presented the first *ab initio* calculation of recombination of BeH^+. At the present stage of the calculations, the results suggest that BeH^+ would recombine very slowly. However, when the nonadiabatic couplings are included, the recombination cross section is believed to increase.

Ursel Fantz: "Fundamental Data of Diatomic Molecules Rel.evant for Fusion"

Ursel Fantz presented results from the Max-Planck-Institut für Plasmaphysik, Garching, Germany. Fundamental molecular data for plasma edge modelling have been compiled. Wherever needed, calculations have been carried out to obtain a data set for hydrogen compounds and isotopomeres. Emphasis was placed on proposed different wall materials in fusion devices such as C, Be and B as well as the recycling molecular hydrogen product. Vibrationally resolved Franck-Condon factors and transition probabilities have been calculated for transitions among electronic states of molecular hydrogen and its coupling to the ground state of the molecular hydrogen ion using the TraDiMo code. For hydrocarbon species CH and C_2 as well as BeH and BH, calculations have been carried out for optical transitions relevant to fusion.

Vibrationally resolved cross sections and rate coefficients for electron impact collisions are compiled from literature and, if not available, calculated using the IPProg code, which is based on the Impact Parameter method. Wherever possible a comparison between calculated and compiled data is made. Data for H_2, CH and C_2 were presented. These data serve as basis for collisional radiative modelling by means of the flexible Yacora code. Calculated and measured photon emission coefficients were also presented. Analyse of mechanisms for population and de-population give insight into relevant processes for the plasma edge of fusion devices.

The relevance of heavy particle collisions in plasma edge modelling has been addressed by adopting the flexible Yacora solver for the dissociation modelling of hydrocarbons. Similar calculations have been carried out for the ion species of molecular hydrogen and the consequences for the analysis of the radiation of atomic hydrogen.

Ratko Janev: "New Contributions to A+M Databases for Fusion Plasma Modelling"

Ratko Janev reported on new theoretical cross-section results for the following collision processes:

1. Vibrational resolved electron impact excitation of CH molecule to A, B and C electronic states
2. Dissociative electron attachment on $H_2(v)$ in the 14-eV energy region
3. State-selective electron capture in H^+, H^{2+}, O^{8+} - H(1s) and He^{2+} - He^+(1s), He^+(2s) collisions
4. Total electron capture in Li^{q+}, C^{q+} - H, H^+ collisions (q = 0 – Z)

Mario Capitelli: "Elementary Processes, Thermodynamics and Transport of H_2, O_2 and N_2 Plasmas"

Mario Capitelli reported on several studies performed at the Bari University and CNR IMIP on the elementary processes, thermodynamics and transport of H_2, O_2 and N_2 plasmas.

The following elementary processes were detailed:

- State-to-state recombination rates calculated by QCT (quasiclassical trajectory) method on the reactions M+M+M = M_2(v,j)+M with M = H,D,O,N. M_2(v,j) represents a molecule in the v^{th} vibrational and j^{th} rotational level,
- State-to-state recombination rates calculated by a semiclassical approach for the recombination rates of atomic hydrogen on graphite (C_g) i.e. the reaction H+H+C_g = H_2(v,j)+ C_g

For thermodynamics, Capitelli reported on a recent study of the influence of calculated partition functions of atomic hydrogen, where electronic levels are calculated using Debye potential instead of Coulomb in the Schrödinger equation.

New calculations of transport cross sections of low- and high-lying excited states of atomic H, N and O were reported. High-lying excited states have a strong influence on the transport properties of LTE

hydrogen plasmas, and the cut-off criterion should be carefully selected to avoid divergence of the partition function.

Model development is in progress for kinetics to simulate a RF Garching discharge for the production of negative ions to be used for neutral beam injection in ITER. The importance of elementary processes was underlined.

Hiroshi Tanaka: "Summary of the Electron Collision Data of C-H and C-F Compound Molecules for Plasma Modelling"

Hiroshi Tanaka presented a comprehensive data compilation for polyatomic molecules relevant to fusion plasma modelling. The main data are differential cross sections and total cross sections for the following processes:

1. elastic electron scattering (differential cross sections)
2. electron induced-resonant vibrational excitation
3. electron-impact excitation of electronic states

Recent results were detailed on the following topics:

1. vibrational excitation functions for inelastic and super-elastic electron scattering in the ground-electronic state in heated (hot) CO_2 molecule
2. electron-impact excitation of the $B\ ^1\Sigma^+_u$ and $C\ ^1\Pi_u$ electronic states of H_2
3. absolute Elastic Differential Cross-sections for Electron Scattering by $C_6H_5CH_3$ and $C_6H_5CF_3$ at 1.5-200 eV: comparative experimental and theoretical studies with C_6H_6

Dr. Tanaka summarized his research activities within the scheme of the CRP, and presented future projects relevant to fusion energy research at Sophia University.

Brendan McLaughlin: "Electron Collisions with Small Molecular Hydrides"

Low energy electron collisions with small molecular hydrides are currently being investigated for a number of different complexes using the state-of-the-art R-matrix method. Elastic and inelastic cross sections for such systems as BeH, BeH_2, CH and CH_2, are all relevant for plasma modeling. Brendan McLaughlin presented a report on calculations for a sample of such molecules.

Jonathan Tennyson: "R-matrix calculations of electron-molecule collisions: scattering from hydrocarbons"

Jonathan Tennyson presented the results of recent calculations at the Department of Physics & Astronomy, University College London. These calculations have considered elastic and electronically inelastic calculations on carbon containing species. Many of the calculations were performed using the automated R-matrix expert system Quantemol-N.

R-matrix studies on electron collisions with acetylene show good agreement with parallel studies performed with a DFT based method. Inclusion of polarisation effects are crucial in both cases to the characterisation of the dominant shape resonance. Calculations were performed for electron collisions with methane, ethane and propane. A 64-state study for methane reproduces the observed Ramsauer minimum, and gives good agreement for total and different cross sections when compared with experiment. This agreement is not reproduced for studies on ethane and propane; this is likely due to incomplete inclusion of polarisation effects.

Calculations on electron impact detachment of C_2^- anions show that this use of the molecular R-matrix with PseudoStates (RMPS) method is able to resolve such problems. However such calculations are not yet possible for complicated molecules. Continued work in this direction is being pursued at UCL.

Khaled Hassouni: "Modelling dust formation in carbon-containing discharge plasmas"

K. Hassouni was not able to attend the meeting. He sent an abstract of his work performed and quoted below. His power point presentation is also available on the A+M Data Unit website.

"The work performed at CNRS-LIMHP is related to the investigation of the molecular growth that leads to the production of carbon particles under discharge conditions. Of special interest are situations where the molecular growth is initiated by small molecular species, typically, C, C_2 and C_3, that are emitted by graphite surfaces submitted to fluxes of ions and active neutral species produced in argon discharges.

This work involves a theoretical aspect where a model couples a discharge physics module, a molecular growth kinetics module and an aerosol dynamic module. Results showed that a significant molecular growth is only possible if clusters and particles are trapped in the discharge. This requires enhanced attachment kinetics and formation of negative clusters in the laboratory investigation.

The formation and molecular growth of hydrocarbon through sputtering and erosion of graphite target were investigated experimentally. Up to 4 carbon hydrocarbon species were detected and it was shown that redeposition can easily take place when graphite is submitted to Ar/H_2 plasmas."

Detlev Reiter: "**Collisional-radiative and Transport Modelling for ITER"**

D. Reiter, R. Janev and B. Küppers

Institut für Energieforschung - Plasmaphysik, Forschungszentrum Jülich GmbH, EURATOM Association, Trilateral Euregio Cluster D-52425 Jülich, Germany

Typically, are encounters equilibria in magnetic fusion plasmas that have been established mainly by the transport flows due to steep gradients and other thermodynamic forces, i.e. "transport equilibria". However, these latter may be significantly modified by atomic, molecular and radiative processes.

Analysis of fusion plasmas, either by plasma diagnostic methods or by numerical simulation, requires one to separate the (assumed known) atomic and molecular effects from the often unknown transport effects. CR equilibrium models are used to separate the fast atomic and molecular processes from the typically much slower transport processes, by dividing up the involved species (their charge states, excitation states) into a subset of "fast" states, which can be assumed to be in quasi steady state (QSS) and a much smaller number of "slow" species, whose distributions evolve only on a time-scale comparable to the transport scale.

After a short introduction to the operational conditions expected in the ITER divertor, Detlev Reiter reported on the status of the hydrocarbon break-up-model as implemented in the HYDKIN online cross-section database and analysis tool. A newly developed interface to the EIRENE transport code, and recent extensions of this tool were discussed, in particular generalization of the online sensitivity analysis.

Major remaining open data issues with respect to hydrocarbons in fusions plasmas were also summarized.

Results Achieved

During the Tuesday afternoon session and Wednesday morning session, the work plan was thoroughly reviewed and results analyzed. Areas that require further investigation were identified. Jonathan Tennyson undertook the task of rapporteur.

This CRP focuses on the gathering and generation of 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. Each participant reviewed their proposed tasks (*in italic*) and summarized the work achieved within the CRP. Every participant commented on and suggested further investigation fields for future CRPs as the discussion unfolded.

Surface processes

Include low-energy D and chemical reactions for C → C_3 hydrocarbons at 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 [Herman].
Achieved: For $C_nD_m^+$ (n = 1, 2, 3) hydrocarbons, ion survival probability, energy transfer to solid, fragmentation and chemical reactions at surfaces, as well as collision kinematics were studied with the following conditions and surfaces:

- at room-temperature and 600° over the incident energy range 15-50 eV for collisions on C, Be and W surfaces,
- at lower energies of 2-10 eV, measurements on heated Be surfaces were completed,
- complete measurements of ion interaction on chemically modified diamond (O-terminated and H-terminated) surfaces were performed.

Cross correlations between all measured ion survival probability data on the different surfaces (C/Be/W) were thoroughly depicted.

*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 [Schultz, Reiter].*
Achieved: The database of Sharma et al has been included in the HYDKIN online analysis tools (http://www.hydkin.de). Sensitivity analysis is not yet completed for surface processes, but was performed for all other data. D. Humbert will collaborate with R. Janev and D. Reiter to incorporate these data into ALADDIN.

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].
Achieved: Experiments are on-going and mass spectrometry studies have already produced preliminary results. A PhD student is currently working on the detailed investigation of the fate of sputtering/erosion products in several discharge or post discharge conditions.

Most basic hydride - study recombination of atomic H/D onto graphite to understand formation of vibrational excited molecules [Capitelli].
Achieved: Studies on graphite, including isotopes is complete. The work on W and Fe is continuing. Difficult to find potential energy surfaces for H/H_2 interactions with Fe and W surfaces. Some preliminary results are available for Fe.

Volume processes

Scheme:
QC → scattering theory/experiment → experimental validation (spectroscopy, fusion experiments) → relevant fusion applications (ITER)

Calculate ground state potential energy surfaces (PES) for hydrocarbons to C_2H_6 [Braams].
Achieved: Potential energy surfaces up to C_3H_4 have been calculated, and some results will be refined. All PES, including C_3H_5, will be fully documented as part of the final report: stationary points, method of calculation, etc.

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].

Achieved: A proposal to study the collisions of H atom with charged hydrocarbons on ground state PES (H extraction: $H + C_mH_n^+ \leftrightarrow H_2 + C_mH_{n-1}^+$) has been submitted to DoE. This does not consider charge exchange, so excited states need to be considered. This study will require much more work; the aim will be to consider reactions on coupled ground and (single?) excited state so that charge exchange can be accounted for at the same time.

Complete the database of e-collision cross sections for vibrational excited molecules (D_2, DT, T_2), and continue work on atom-diatom, electron-molecule collisions. Carry out a benchmark comparison with R-matrix results at lower energies. For the atom-molecule collisions, compare the results with the data from Krstic et al. for H-H_2 and H^+-H_2 collisions. [Capitelli]

Achieved:

- electron-H_2 isotopologues database is complete for vibrationally resolved transitions from X state to singlet excited states. Also included are some triplet –triplet transitions with $n < 4$.
- The work for atom-diatom is completed, including a scaling law for isotopologues. The cross sections for elastic and dissociation for H-H_2 and H^+-H_2 collisions look very similar. Fits are available for the rate coefficients, and are in progress for the cross sections.
- Electron-molecule: new results are available for the 14-eV resonance process DA including dependence on v and J. The calculations are vibrationally resolved for H_2.
- The comparison with R-matrix dissociation cross sections is completed: differences approach a factor of two in rates, the R-matrix results are usually higher. The database uses an analytic form for these cross sections up to v = 14.

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

Achieved: Ionization energies for BeH, BeH_2 up to Be_xH_y ($x<5$, $y<10$), including atomization and dissociation energies, were calculated. BEB (Kim) total ionization cross section will be calculated for these systems.

The four topics listed below involve Dr. Kimura. Some results were submitted at the second RCM. Dr. Tanaka will contact Kimura's collaborators to provide results, so that D. Humbert can incorporate them into the ALADDIN database.

Calculate excited state molecular structure up to C_4H_8.
Evaluate CO sticking on metallic substrate surfaces (Ag) [Kimura].

Achieved: STET completed electronic structure calculations on hydrocarbons.

Undertake nuclear motion calculations and identification of fragmentation pathways on excited states. Perform CO sticking and desorption calculations.
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].

Achieved (June 2007): completed calculations on C^+ at higher energies.

Extend calculations to lower collision energies [Kimura].

Achieved [R. Janev]: Calculated cross sections for H atoms with fully stripped ions (He^{2+} to O^{8+}) are complete using atomic orbital close-coupling over large basis sets of energy range from 0.2 to 200 keV/u.

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

Achieved (June 2007): CH_4 and C_2H_2.
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). Complete studies and include vibrational effects correctly. Consider CH^+. [Tennyson, McLaughlin].
Extend range (energy and geometry) of electron H_2 studies [Tennyson].
Evaluate electron–C atom collisions (elastic and momentum transfer cross sections)? [McLaughlin]
Achieved:

- Elastic and inelastic collisions with C_2, and elastic electron collisions with HCCH were also evaluated [Tennyson].
- Work on BeH and BeH_2 is completed. The electronic excitation for BeH is anomalously small; Born corrections are probably needed [McLaughlin].
- CH studies: CH structure is complete, collisions are in progress. Vibrational excitation and isotope effects will follow [McLaughlin]. Electron impact excitation (smoothed interpolation of R-matrix data at low energy and Born at high energy) of CH with scaling for vibrational states are available [Janev].
- electron–C atom collisions: NASA compilation of momentum transfer cross sections shows a factor of 4 to 5 between C and N, O. Results will be re-evaluated with existing studies [McLaughlin].
- Electron H_2^+ resonance parameters have been computed for extended energy and geometry. Extension to energy dependent resonance widths is in progress.
- Electron H_2 collision studies for extended energy and more electronic states in progress at UCL.
- Electronic excitation of HCCH (and methane) is complete [Tennyson].
- CH^+: a new project has started at UCL.

Benchmark C_2H_2 rates, electron collision cross-sections.
Elastic, vibrational and electronic excitation (break-up) [Tennyson, McLaughlin, Tanaka].
Achieved: Experimental elastic and vibrational excitation cross sections are available. Calculated elastic cross sections are complete. More theory and experiment for electronically inelastic cross sections is needed. Results for methane are available, and may possibly be published in APID.

Ionization data for C_2H_2 [Braams, used as input by Hassouni].
Achieved: Calculation of the ionization threshold for C_3H has been performed. Ionisation data are available in standard databases (eg CCCBDB at NIST). Investigation on the effect of vibrational distributions in plasmas on processes such as near threshold ionization of HCCH is needed.

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 modelling at Jülich, and updating of the database [Tanaka et al].
Achieved:
1) **EELS (Electron Energy Loss Spectroscopy)**:

- Electron elastic scattering DCS on C-H and C-F compounds were measured. The molecules studied include C_3H_6 isomers, CF_3X (X = Cl, Br), CH_3X (X=F, Cl, Br, I), C_6H_5X (X=H, CH_3, CF_3) and 1,1-$C_2F_2H_2$. Generalized Oscillater Strengths were calculated for CO, H_2, CO_2 and N_2O applying the *BEf* scaling law.
- Absolute vibrational excitation DCS from vibrationally excited molecules for CO_2 and N_2O by electron impact are available.

2) **QMS (Quadra-pole Mass Spectroscopy)**:

- Absolute total cross sections for the neutral non-emissive radicals of CH_3 from CH_4 by electron impact from threshold to the ionization energy region were measured.

- The negative ion formations (resonant dissociative attachment) of CH_3^-, CH_2^-, CH^- and C^- were verified using a new QMS system.
- Formation of SiH_3^-, SiH_2^-, SiH^-, Si^- from SiH_4 as well as GeH_3^-, GeH_2^-, GeH^-, Ge^-, from $GeiH_4$ by electron impact were measured.

3) **Database**: compiled data are:

- Elastic DCS of polyatomic molecules by electron impact.
- Cross sections of electron-induced resonant vibrational excitations in polyatomic molecules.
- Electron-impact excitation cross sections of electronic states in polyatomic molecules.

The database compiled in NIFS report of 2007 (*Database for Electron Collisions with Polyatomic Molecules: Elastic-, Resonant Vibrational- and Electronic Excitations*) will be revised and submitted to the IAEA. New results will be published either in the IAEA APID series or another publication.

Further calculations and measurements are on-going:

- **EELS**: clean W, Be, and C surfaces, as the targets for electron collision, have been employed to determine the ratio of elastic and inelastic scattering of electron from these surfaces.
- **QMS**: formation by electron impact on methane of neutral non-emissive (dissociative) radicals CH and CH_2 is being measured in the threshold region.

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

Achieved: 80+% of H data now exist in HYDKIN, the remaining data are being entered. At present time, no rotational information/temperature is available. HYDKIN is being continuously updated with data from this CRP and elsewhere. Humbert, Reiter, Janev and Clark will collaborate to provide on-line HYDKIN data using either the IAEA search engine GENIE or the ALADDIN database.

C_3H_x ionic systems - recombination, and dissociation excitation – cross sections and rate coefficients. Evaluate relevance of BeH^+, BeH_2^+ and perform calculations on BeH and DR on CH_4^+ [Larsson]. Explore effect of target temperature [Schultz]

Achieved:

- Measurements and calculations for C_3H_4, C_3H_7, C_4D_2, D_2H^+ and BeH^+ have been carried out. The rate coefficients are low for BeH^+. Non-adiabatic mechanisms will be investigated.
- CH_4^+ DR is outstanding.
- Target temperature effects are hard to include in models as the data are insufficient. Many more state-selective results are required.
- Measurements on Be have not been undertaken because CRYRING is unable to handle such a system.

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

Achieved:

- Partial cross sections for ionization and appearance energies for ionization have been measured for C_3H_8, C_2D_6, CD_4, CH_3D, C_2D_6, C_3H_8 and $C_3H_6D_2$ at room temperature and 700K. Measurements for methane, ethane, C_2H_4 and C_2H_6 are in progress. [Matejcik]
- All new data are regularly incorporated into a PIC/MCC model to simulate the CASIMIR device behaviour. [Hassouni]

Carry out CR modelling using data from Bari for H_2 (D_2). Investigate differences in excitation for isotopes. Validate for HD in ECR discharges. [Fantz]

Achieved: Tools are available for H_2. Additional required data will be provided by Capitelli. Preparation of the full D database is well underway. Comparisons between H and D were made by means of measurements, and no strong effect was observed.

Carry out CR modelling for C_2/CH molecules. FC factors, systematic transition probabilities are required. A CR model for BeH and BH is of high interest for diagnostic applications. [Fantz]

Achieved: the CR model for C_2/CH is operational, and includes 10 electronic, vibrationnally-resolved levels for C_2 and 4 levels for CH. FC factors and transitions probabilities are available for C_2, CH, BeH and BH, as well as for D and T isotopologues. Matejcik will provide highly-accurate structure data for BeH. Approximations made for CH data will be checked using R-matrix data from McLaughlin. BH is of low priority.

Carry out CR/dissociation modelling to determine PECs for CH, C_2 and H_2 to test available databases, and to 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].
Achieved: Measurements have been performed, and the models do not reproduce all observations. Sensitivity studies for chemistry were performed with current databases.

Extend the 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].
Achieved:

- Experiments are underway with pure H and graphite target.
- PIC model is now operational for H_2 discharge with detailed hydrogen kinetics (vibration, attachment, ionisation, electronic excitation, etc.). Hydrocarbon chemistry is now being incorporated into the model.

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].
Achieved:

- CR model was successfully applied to experiments at University of Augsburg, ASDEX Upgrade and negative ion sources at IPP. Problems with CR model were identified. Treatment of H_2^+ and H_3^+ DR and mutual neutralization (H- with H_2^+, H_3^+) were highlighted as issues and improved.
- A full hydrogen CR model has been developed and included in PIC model to simulate CASIMIR. This model was used at the University of Bari to test the sensitivity of simulation results to different plasma models [Diomede et al. *Phys. Plasma* 15(10), (2008)]

Investigate use of line shapes (CH, C_2 and C) to give information on kinetics of break-up [Fantz].
Achieved: Laboratory measurements show two rotational temperatures due to break up dynamics. Further investigations have low priority.

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].
Achieved:

- Studies of break-up kinetics extended to C ions have been performed.
- J-R/E-L databases have been compared.
- Greifswald data were added to HYDKIN. Alman-Ruzic data still need to be added with possible overlap with the already available data in HYDKIN.

Applications to JET and ITER are on-going. More cross sections are still required in the CR model for atomic C as well as data on fragmentation of hydrocarbons at surfaces.

Hydrocarbon molecular ion reactions: [Schultz,Bannister]
Achieved:

- Measurements of electron-hydrocarbon molecular ion reactions (DE, DI, ionization) at ORNL have been collected, and plans to continue this work have been made in order to test and extend the existing database.

- A preliminary molecular dynamics-energy deposition model has been developed to treat a wide range of electron-hydrocarbon molecular ion dissociative processes. This model has been applied to e + CH+ as a test case.

Publication of Results and Data Collection

The results of the CRP will be published in a new volume of the Atomic and Plasma-Material Interaction Data for Fusion (APID) Series dedicated to the CRP, with each participant submitting a paper. An introduction to the APID issue will be written by staff of the A+M Data Unit. Papers should be 15 to 20 pages in length, including graphics. A general layout of the article was distributed (see Annex 3).

A primary aim of the A+M Data Unit is to established numerical databases for use in fusion energy research. Participants will provide numerical data from the CRP in an electronic form to be included in the IAEA AM/PSI ALADDIN database. Only AM collisional data (cross sections and rate coefficients) and PSI data are currently included in ALADDIN. Other data may be placed on-line at different data centres, such as NIST for spectroscopic data or at NIFS. Submitted data should satisfy the following criteria:

- Raw data are preferred to filled data. Errors bars are essential.
- Process, reactants and products should be clearly identified.
- Method and bibliography sources should be specified (if data already published).
- An estimation of the accuracy of the data is essential.

Data can be provided in a single file or split into different files, as long as the data can be parsed easily electronically.

Agreed deadline to submit papers and to provide data is 15 January 2009.

Recommendations and Future Developments

The detailed list of outputs and further tasks to be performed reveal a number of areas that merit further investigation with respect to both surface and volume processes.

The CRP did not have enough expertise to address many of the issues identified with surface processes. These areas could be addressed during the course of the CRPs on “surfaces erosion” and “formation of dust in tokomaks reactors”. Close collaboration between these CRPs is highly recommended. Participants highlighted two important issues:

- The effect of molecular vibrational distributions is not known, and difficult to address experimentally.
- In what form does berrylium leave the surface?

Areas which would benefit from further investigation to quantify volume processes are:

- Full quantal test for H+ ↔ hydrocarbon collisions, with Langevin rates (particularly at energies below 2 eV) of high interest.
- There is a need for a complete deuterium database, including DA of D_2, DR of D_2^+ and D^+, D_2 collisions. Also reliable (quantal) vibrationally-resolved cross sections for H and H_2 collisions are needed (e.g. VT transfer, excitation) as a check on semi-classical calculations. Isotope effects must be considered.
- Electron impact excitation cross sections of H_2 X state to triplets (with n up to 3) vibrationally resolved, with an electron temperature up to 10 eV. Beyond n = 3, a scaling law may be used.

- Vibrational effects in electron-C_2 collisions are important. Some geometry-dependent data are already available.
- The BeH/BeD emission spectra are not well understood and need further investigation.
- Vibrationally-resolved electron impact electronic excitation data are required for BeH (BeD, BeT), CH (CD), BH (BD), as well as for dielectronic recombination data for CH_4^+.
- Electron impact electronic excitation (both dissociative and non-dissociative) cross sections are needed for hydrocarbons. Measurements are possible using photon emission for hydrocarbons.

At Sophia University, Tokyo, Japan, the measurement of new C-H compounds, H_2 and D_2 data by two new experimental facilities is still an active project:

- Two EELS systems continuously and systematically provide DCS for plasma-relevant C-H compounds.
- Temperature and surface material effects on the cross section are studied by comparing cross sections of vibrationally-excited molecules of H_2* and D_2* colliding with electrons emitted from W, Be, and C filaments.
- Electron-molecule collisions data (C_2H_2, CH_4, and C_2H_4) are measured to validate usage for the *BEf* scaling law.
- More reliable total cross sections for simple C-H compounds are measured down to 10 meV, with very low-energy photoionization from Ar by the SR.
- Excitation cross sections for the electronic states are measured near the threshold by the TOF technique.
- Neutral C-H radical production from the simple C-H compound molecules are measured by means of threshold ionization spectroscopy.

Stockholm University, Sweden, possesses the expertise and facilities for electron molecular ion scattering calculations. Measurements on anion-cation collisions are possible.

Conclusions

The CRP on “Atomic and molecular data for plasma modelling” focused on gathering and generating new data relevant to the edge region of plasmas in nuclear fusion energy devices. This CRP has been particularly successful in generating new data essential for the modelling of the plasma edge region, as well as in surface processes as well as volume processes.

All results will be published in a new volume of the Atomic and Plasma-Material Interaction Data for Fusion (APID) Series devoted to the CRP. New collision data are being collected and introduced into the IAEA AM/PSI ALADDIN Database. Data needs were also identified in a number of areas that will greatly benefit from further research.

Appendix 1

IAEA Final Research Coordination Meeting: Atomic and Molecular Data for Plasma Modelling

17–19 November 2008, Building-A, floor-07, room-42 (A07-42), IAEA Heaquarters, Vienna, Austria

Scientific Secretary: Denis Humbert

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Appendix 2

IAEA Final Research Coordination Meeting: Atomic and Molecular Data for Plasma Modelling

17–19 November 2008, building-A, floor-07, room-42 (A07-42), IAEA Heaquarters, Vienna, Austria

Scientific Secretary: Denis Humbert

MEETING AGENDA

Monday, 17 November

09:15 – 09:45	Opening, Adoption of Agenda, A. Nichols, R.E.H. Clark, D. Humbert	
09:45 – 10:00	Homage to Dr. Kimura	

Session 1: Current Research

Chairman: M. Capitelli

10:00 – 10:45	Z. Herman	Interaction of slow ions with surfaces: Ion survival probability on carbon, tungsten and beryllium surfaces (room temperature and heated)
10:45 – 11:15	*Coffee Break*	
11:15 – 12:00	D. Schultz	Electron-hydrocarbon molecular ion reactions
12:00 – 12:45	S. Matejcik	Electron impact ionization studies of small hydrocarbons and beryllium compounds
12:45 – 14:00	*Lunch*	

Session 2: Current Research (continued)

Chairman: B. McLaughlin

14:00 – 14:45	B. Braams	Potential energy surfaces and applications for hydrocarbons
14:45 – 15:30	M. Larsson	Progress report: Calculations on BeH^+
15:30 – 16:00	*Coffee Break*	
16:00 – 16:45	U. Fantz	Fundamental data of diatomic molecules relevant for fusion
16:45 – 17:30	R. Janev	New contributions to A+M databases for fusion plasma modeling

Tuesday, 18 Novemeber

Session 3: Current Research (continued)

Chairman: U. Fantz

09:00 – 09:45	M. Capitelli	Elementary processes, transport and kinetics of H_2, N_2 and O_2 plasmas
09:45 – 10:30	H. Tanaka	Summary of the electron collision data of C-H and C-F compound molecules for plasma modeling
10:30 – 11:00	*Coffee Break*	
11:00 – 11:45	B. McLaughlin	Electron collisions with small molecular hydrides
11:45 – 12:30	J. Tennyson	R-matrix calculations of electron-molecule collisions: scattering from hydrocarbons
12:30 – 14:00	*Lunch*	

Session 4: Current Research (continued)

Chairman: R. Janev

14:00 – 14:45	D. Reiter	Collisional-radiative and transport modeling for ITER
14:45 – 15:15	*Coffee Break*	
15:15 – 17:00	All	Summary of current research

Wednesday, 19 November

Session 5: Summary of CRP Results

Chairman: B. Braams

09:00 – 11:00	All	Data compilation, production and evaluation. Database additions
10:45 – 11:15	*Coffee Break*	
11:15 – 12:30	All	Discussion continued
12:30 – 14:00	*Lunch*	

Session 6: Recommendations from CRP and Conclusions

Chairman: R.E.H. Clark

14:00 – 16:00	All	Conclusion and recommendation for new CRPs
16:00 –	*Adjournment of Meeting*	

General Layout of APID Documents

Ask authors to look at http://www-pub.iaea.org/MTCD/publications/PDF/APID-Vol13_web.pdf for style.

The main points are:

i) Run a spell check (UK English)

ii) Titles, sub-titles and sub-subtitles *ad infinitum* will be put into the form detailed below, so we would be grateful if authors can avoid inappropriate capital letters and bear the numbering convention in mind. The problem we have had in the past is that when some authors put their titles into capitals, when we imposed the style it was not always clear to the non-initiated how ASDEX or JET etc should be written. Authors don't need to worry too much about the minutiae like italics, if they forget will be sorted, but capitals are a pain as are numbering systems with letters or Roman numerals which are referred to in the text.

Paper title, (upright, bold, first letter caps)

Abstract, References (upright, first letter caps, un-numbered)

1. Sub-title, (upright, first letter caps, note the period)

1.1. *Sub-subtitle,* (italics and first letter caps, note the second period)

1.1.1. *Sub-subsubtitle* (italics and first letter caps, note the third period)

See page 10 of http://www-pub.iaea.org/MTCD/publications/PDF/APID-Vol13_web.pdf for good examples.

iii) Affiliations in the form:
Name A[1]*, Name B*[2]*, Name C*[3] ...(italic and superscript numbers)

[1]Lawrence Livermore…

iv) Figure Captions
Figure 1. Caption, caption, caption.. (Figure not Fig. **Figure 1.** in bold, upright. Note the period. Caption in upright, first letter caps). Numbers not Roman Numerals or A, B etc.

v) Table Captions
Table 1. Caption, caption, caption.. (**Table 1.** in bold, upright. Note the period. Caption in upright, first letter caps). Numbers not Roman Numerals or A,B etc.

vi) Authors should endeavour to supply equations pre-split to a size appropriate for a double column format

vii) Try to use software that turns equations into pictures to avoid symbol changes on typesetting.

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