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XSAMS: XML Schema for Atoms, Molecules and Solids

Summary Report of an IAEA Consultants' Meeting

National Institute for Fusion Science

Toki-Shi, Gifu-Ken 509-5292, Japan

24-26 March 2010

Prepared by

B J Braams
International Atomic Energy Agency, Vienna, Austria

May 2010

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Abstract

Experts on atomic and molecular data and their exchange met at National Institute for Fusion Science, Toki-City, Japan, to review progress in the implementation of XSAMS, the XML Schema for Atoms, Molecules and Solids, and to discuss further development of the Schema. The proceedings of the meeting are summarized here.

May 2010

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1. Introduction

During the past decade XML (Extensible Markup Language) has emerged as an important tool for electronic information exchange. In October 2003, development of a new XML-based standard for exchange of atomic, molecular, and particle-solid-interaction data was proposed at the IAEA Data Centre Network meeting. At the same time, similar needs were recognized by other researchers, in particular within the International Virtual Observatory Alliance (IVOA). This led to an international collaboration of which at this time the core institutions are the IAEA, the National Institute of Standards and Technology (USA), Oak Ridge National Laboratory (USA), the Université Pierre et Marie Curie and Observatoire de Paris Meudon (France), the Russian Federal Nuclear Center All-Russian Institute of Technical Physics and the National Institute for Fusion Science (Japan). The goal of this project is to develop an XML Schema for Atoms, Molecules and Solids (XSAMS) and to encourage its use as a language for querying and retrieving information from atomic, molecular, and plasma-material interaction (A+M/PMI) databases. The first release of XSAMS, version 0.1, took place in September 2009. The document is here: http://www-amdis.iaea.org/xsams/documents/.

The IAEA has supported the development of XSAMS through its Data Centre Network meetings and through dedicated Consultants' Meetings. The most recent Consultants' Meeting on XSAMS took place 24-26 March 2010 and the proceedings of that meeting are summarized here. With a view towards outreach for the XSAMS project and broader A+M/PMI activities it was found attractive to organize the meeting this time at a location other than IAEA Headquarters. The IAEA is grateful to the National Institute for Fusion Science (NIFS) and to Dr Izumi Murakami of NIFS for hosting the meeting, which was well attended by scientists from Japan and neighbouring countries.

On Wednesday morning 24 March a tour of NIFS was provided, including a show of the Large Helical Device stellarator experiment by Dr Motoshi Goto and of the CompleXcope virtual reality center by Dr Shunsuke Usami and Dr Masahiko Sato. The meeting proper commenced Wednesday afternoon. On Wednesday afternoon and Thursday morning participants provided overviews of their data center activities, with special interest in XSAMS, but not limited to the Schema. Also a tutorial presentation on XSAMS was given. On Thursday afternoon and even more so on Friday there were further presentations, but they served mainly to guide technical discussion as the meeting turned into a working meeting among those involved in the further development of XSAMS. Meeting presentations are collected on the A+M Data Unit XSAMS web pages at http://www-amdis.iaea.org/xsams/executive/.

Section 2 of this report provides a summary of the presentations of Wednesday afternoon and Thursday morning. Section 3 presents the discussions of Thursday afternoon and Friday morning and the work plan. Section 4 provides conclusions. The list of participants is provided in Appendix 1 and the meeting agenda in Appendix 2.

2. Summary of Presentations

Dr Motoyasu Sato, Director of the Coordination Research Center at NIFS, and Dr Izumi Murakami, head of the Atomic and Molecular Data Research Center within the Coordination Research Center and local organizer of the meeting, welcomed the participants. They noted the importance of XSAMS for data exchange and expressed the hope for a successful meeting. Dr Bas Braams, scientific secretary of the meeting, added his welcome and requested approval of the report of the previous meeting, 10-11 September 2009 at IAEA, and of the agenda (see Appendix 2). It was noted that Dr Yongjoo Rhee of KAERI (Korea) attended the previous meeting, but his name is missing from the list of participants there. With that correction the report of the previous meeting was approved, as was the agenda.

Dr Izumi Murakami then described the work of the Atomic and Molecular Data Research Center at NIFS (web page at http://dpc.nifs.ac.jp/amdrc/). The Center develops and maintains its own original numerical databases and they offer a portal, in some cases through their own interface, to additional numerical and bibliographical databases. The main point of entry is https://dbshino.nifs.ac.jp/ and the

databases can be freely accessed from there without registration. Among the numerical databases AMDIS is by far the largest, containing more than 400,000 records as of February 2010. AMDIS has subsections EXC, ION and REC for electron impact excitation, ionization and recombination of atoms, and DIO for electron impact dissociation of molecules. Other, much smaller numerical databases are CHART for charge transfer in ion-atom collisions, AMOL for electron collisions with molecules, CMOL for heavy-particle collisions with molecules, and SPUTY and BACKS for sputtering yields and reflection coefficients for collisions on solid surfaces. A Data Update working group consisting of atomic and molecular physicists in Japan and NIFS staff carries out critical compilation of data published in journals for entry into AMDIS, CHART, AMOL and CMOL. The bibliographical atomic collision database at NIFS is derived from the one developed and maintained at Oak Ridge National Laboratory, but it has a different user interface than at ORNL and it offers cross-references to the numerical databases. Finally, through the dbshino web entry point one finds mirror access to several further numerical databases not developed at NIFS.

In recent years there are about 5,000 search accesses per year of AMDIS and over 7,000 per year for all the numerical databases together. In her talk Dr Murakami showed the web interface for the principal databases; for this, please see her presentation under http://www-amdis.iaea.org/xsams/executive/. It is planned to migrate all the databases into a new system in the course of 2010; this is necessary because the support contract for the present database system expires and will not be renewed. It is an occasion to reconsider the organization of the databases and perhaps create a completely new system and a new interface for easier use. This would be the start of a long term project, and one aspect of the new system may be to use XML/XSAMS for output.

Dr Masatoshi Ohishi of the National Astronomical Observatory of Japan (NAOJ) described work of the International Council for Science (the ICSU, previously known as the International Council of Scientific Unions) on approaches to management of scientific data. The ICSU (http://www.icsu.org) is a non-governmental international organization founded in 1931. It has 119 national member societies and 30 international scientific union members. The International Astronomical Union is a member. The traditional focus area of the ICSU is earth and solar science, and it is increasingly concerned with environmental science. In the field of scientific data management and use the best known activity of ICSU is CODATA, the Committee on Data for Science and Technology. The ICSU maintained a network of World Data Centers to facilitate international data exchange and to develop data management plans for separate disciplines. In 2008, considering the changes in world-wide electronic connectivity and the end of the cold war, it was decided to replace these Centers by a World Data System (WDS), which also incorporates the activities of the Federation of Astronomical and Geophysical Data Services (FAGS; http://www.icsu-fags.org). Astronomy deals with very large observational datasets that are maintained in "virtual observatories." Dr Ohishi is the lead representative from the Japanese Virtual Observatory on the International Virtual Observatory Alliance (IVOA) and participates from that background in the ad hoc Strategic Coordinating Committee for Information and Data (SCCID) of the ICSU. The SCCID has been established for an initial period of 3 years starting in 2009 and is to provide broad advice about the role of the ICSU in the management and dissemination of scientific data. (See http://www.icsu.org/1_icsuinscience/DATA.html for further information about the WDS and the SCCID.) In initial discussions the SCCID identified 4 successful models for large-scale data sharing: the world-wide Protein Data Bank (http://wwpdb.org), the OneGeology project (http://www.onegeology.org), the Intergovernmental Panel on Climate Change (http://www.ipcc.ch) and the International Virtual Observatory Alliance (http://www.ivoa.net). (It was noted that the IPCC has been under some fire recently.)

In the remainder of his talk Dr Ohishi concentrated on the work of the IVOA, which is concerned with tools, systems and organizational structures for the international shared utilization of astronomical archives. Data resources that are anticipated for IVOA include those of the Atacama (Chile) Large Millimeter/submillimeter Array (ALMA), the James Webb Space Telescope (JWST), the Large Synoptic Survey Telescope (LSST), the Low Frequency Array (LOFAR), the Square Kilometer Array (SKA) radio observatory, the Thirty Meter Telescope, the Giant Magellan Telescope, and the European Extremely Large Telescope. The IVOA successfully produced recommendations for data standardization among these and other projects; see http://www.ivoa.net/Documents/index.html. For

example there are recommendations for meta-data description and its exchange, access protocols to images (Simple Image Access Protocol – SIAP), spectra (Simple Spectrum Access Protocol – SSAP) and catalogues (Table Access Protocol – TAP), a query language to access federated databases (Astronomical Data Query Language – ADQL), a standardized method to describe different attribute names with the same semantics (Unified Contents Descriptions – UCD), and a data query format by means of XML (VOTable). Through its work the IVOA has learned that indeed standards are quite effective in promoting the wider dissemination and use of data; on the other hand, establishing standards is a painful process. Good communication, also outside the formal meetings, among participants in the standardization process is important. Some specific projects were described in more detail: the "VOSpec" spectrum viewer through SSAP developed by the European Space Agency Virtual Observatory and the Data Grid of the Astronomical Virtual Observatories. Evidence of the value of the Virtual Observatory concept is found in the citation indices, with more than 1300 papers in the NASA Astrophysics Data System mentioning "Virtual Observatory" somewhere in the text.

In conclusion Dr Ohishi provided recommendations and lessons learned relevant to our meeting. Technology should be neither too early nor too late; it is important to use stable and robust technology that is platform-independent and already has some popular following. The work should be science-driven, as may be seen through joint publications between data experts and observational scientists. There should be convenient public access to all policies, meeting minutes, standards and other documents. Governance should be assisted by an expert advisory group. Try to schedule meetings in connection with major international meetings and use teleconferencing. Link the domain-specific standards to international standards, such as XML. Use free tools whenever this is feasible. Focus on standards for data exchange rather than database design; leave the database management to the individual participants. Try to use a single portal for user discovery from distributed sources of information. Make data and information available free of charge to all users.

Dr Evelyne Roueff described database work at the Paris-Meudon Observatory, mentioning BASECOL and focusing on MOLAT database. The Basecol project was initiated by Dr Marie-Lise Dubernet when she was still at Observatoire de Paris-Meudon, and she remains the lead person on the collaboration in her new position at UPMC. The project (http://basecol.obspm.fr/) is motivated by anticipated data from the Herschel Space Observatory (HSO) and from the Atacama Large Millimeter/submillimeter Array (ALMA), which will be measuring millimeter and submillimeter (mainly) rotational molecular spectra.

MOLAT contains original atomic and molecular data and compilations produced independently or during collaborations involving members of Paris Observatory. It includes experimental spectroscopic data (mainly VUV) obtained by the Meudon experimental group using either the 10m high resolution VUV spectrograph of the Observatory or the LURE-Orsay synchrotron facility. MOLAT also includes theoretical data from different groups of the Observatory concerning atomic or molecular structures, radiative transition probabilities, electron impact excitation cross-sections of Neon-like ions and Stark broadening parameters. Links to other pertinent atomic or molecular databases are also provided. An effort is underway to give a more unified presentation of these various data. Some of these databases have been processed with use of Virtual Observatory tools. Access to BASECOL and CDMS data via Virtual Observatory tools is described in Dr Dubernet's presentation. A spectral line access protocol has been set up on the theoretical VUV theoretical H_2 data base, allowing to get the relevant information for a given spectral interval on the spectral properties of H_2, HD and D_2 (wavenumbers, oscillator strengths, term energies of the upper and lower levels, corresponding quantum numbers, and other information). The Stark-b database is another example that is concerned with Stark broadening of selected isolated lines of atoms and molecules in the impact approximation according to theoretical calculations. Meudon also contributes to the theoretical TIPTOP database, which is stored at the Strasbourg astronomical Data Center (http://cdsweb.u-strasbg.fr/OP.htx).

Dr Peter Loboda described the atomic data and database activities carried out at the Russian Federal Nuclear Center – All-Russian Institute of Technical Physics (RFNC-VNIITF) in collaboration with researchers from the Joint Institute for High Temperatures of the Russian Academy of Sciences and the P.N. Lebedev Institute of the Russian Academy of Sciences. At VNIITF there is particular interest

in equation-of-state (EOS) calculations and emissions and opacities of hot dense plasma utilizing superconfiguration and also detailed kinetic descriptions of the ionization balance and of the bound-bound and bound-free spectral distributions. This work relies on atomic data calculations for multielectron ions, and the group develops and maintains databases of atomic and opacity data. The models and data are applied to laboratory plasma diagnostics, to modeling of laser-plasma x-ray sources, and to other purposes.

Dr Loboda illustrated the structure of the comprehensive calculations, which has the nature of multispecies chemical modeling. The plasma is treated as a thermodynamic equilibrium mixture of ions with internal degrees of freedom (excited states) and free electrons. The fundamental thermodynamic quantity is the Helmholtz free energy in which there are contributions from an ionic ideal gas, from each charge state of ions with bound electrons, from a partially degenerate free-electron ideal gas, and from the interparticle interactions. Opacities may be calculated by the code Spectr-STA, which relies on a superconfiguration model (STA, Super Transition Arrays) in which transitions between superconfigurations are modelled by effective spectral distributions corresponding to single electron transitions. The ion populations are obtained from modified Saha equations. The Gaussian or Voigt effective line shapes for the transition arrays include statistical energy dispersion and Doppler broadening or radiative plus collisional broadening. Single and two-electron atomic data and configuration properties are calculated by using the RCN36 program from the Cowan suite of codes; this is to be replaced by the FAC-code data in a new version of Spectr-STA. Opacities may also be calculated by the code Spectr-DTA, which relies on a detailed description of bound-bound and bound-free transitions (DTA, Detailed Transition Accounting). Using Spectr-DTA ionization balance and ion state populations may be obtained from superconfiguration ionization balance models and then assuming Boltzmann LTE distribution over detailed terms, or from calculations based on other NLTE collisional radiative models. The calculation of opacities involves finally a density-matrix based approach called LineDM. This model includes the most important line-broadening mechanisms and enables to describe the effect of the plasma microfield and radiation field on the population kinetics of ionic states. The key atomic radiative transition data that are input to these Spectr-DTA calculations are obtained from the GRASP^2 Multi-Configuration Dirac-Fock package and from the Flexible Atomic Code (FAC). Autoionization widths and photoionization cross-sections may be calculated using the distorted wave approach with FAC. A pilot version of the relevant database is being developed and is being filled now with consistent spectroscopic data for multielectron ions.

These calculated data together with assembled experimental and compiled data enter into the Spectr-W^3 database, http://spectr-w3.snz.ru/. Spectr-W^3 contains at this time about 450,000 records of ionization potentials, energy levels, wavelengths, transition probabilities, oscillator strengths, statistical weights, and line shape parameters. The database also offers fitting formulae and fitted parameters for analytical approximations of collision cross-sections and electron transition rates in atoms and ions. The data are linked to bibliographical information and other metadata. The data sources include papers published in leading physical journals, datasets submitted by the authors, and high-resolution experimental and reliable theoretical data obtained by the project participants. The Spectr-W^3 project is supported by the International Science and Technology Centre (ISTC). Under the current ISTC project the Spectr-W^3 database will be enhanced in content and interface; of special note for XSAMS is the intent to provide utilities to export the data in XML format, as well as plain text format and (already in place) HTML format. The Spectr-W^3 group actively participates in XSAMS and a pilot implementation of XSAMS for Spectr-W^3 has already been achieved, as will be presented later in the meeting. The Spectr-W^3 project also collaborates in the Virtual Atomic and Molecular Data Centre (VAMDC) that is coordinated by Dr Marie-Lise Dubernet and of which more is heard at this meeting.

Dr Jung-Sik Yoon presented work that is being done in the Data Center for Plasma Properties (http://www.nfri.re.kr/english/research/plasma_current_04.php?tab=4) in the National Fusion Research Institute (NFRI) in Korea. NFRI is the principal Korean institute for fusion energy research. The large, overarching projects at NFRI are the Korean contribution to ITER and the experimental programme on the superconducting KSTAR tokamak. However, motivated by plasma applications broadly (fusion as well as industrial plasma) NFRI also has a project to construct a plasma properties database and

associated simulation systems. The present status of that project may be seen on the web at http://plasma.kisti.re.kr/, home of the "Atomic and Molecular Database for Industrial Plasma". The site is at this time almost entirely in Korean; however, it is planned to have an English-language web interface in due time. The database is organized as a Knowledge Base and the numerical data are connected to simulation codes on the same site. The principal focus so far is on industrial plasma, for example for etching, and codes available through the site include a particle-in-cell plasma simulation code.

Dr Yoon emphasized the need for evaluated data. Data evaluation includes comparison between different data sets as well as expert tests. Korean Standard Reference Data norms and a guide from ISO-GUM (1993) require certified data with stated uncertainties. Validation can also be carried out at the level of a complete data set, for example by using such a dataset in a full Boltzmann simulation including transport. The work of the data center at NFRI takes place in cooperation with the Asia-Pacific Atomic Data Network. There are prospects for a Global Frontier Project for an International Atomic and Molecular Data Centre, in which the NFRI data centre would participate.

Dr Yuri Ralchenko provided a general introduction to XML schema and XSAMS. (In a subsequent presentation, see below, he described the database work at NIST). The initiative to develop XSAMS goes back to the IAEA Data Centre Network meeting in 2003 where a working group was created to develop an XML Schema for exchange of atomic and molecular data, then under the working name of AMDML. At present development of XSAMS primarily involves people from the IAEA (B.J. Braams and H.-K. Chung), the Observatoire Paris-Meudon and the Université Pierre et Marie Curie (E. Roueff and M.-L. Dubernet), Oak Ridge National Laboratory (D.R. Schultz), VNIITF (S. Gagarin and P.A. Loboda), NIST (Yu. Ralchenko) and NIFS (D. Humbert). R.E.H. Clark and N. Moreau contributed in the past. The web site of XSAMS is http://www-amdis.iaea.org/xsams/.

XML/XSAMS is a mechanism for exchange of data. It has been developed for us, atomic and molecular physicists who need data. Using XSAMS for exchange of data increases the confidence that what is exchanged are real physical data and that they are interpreted correctly; contrast this with exchanging data in the form of ASCII numerical files. XML belongs to a broader view of data handling that is concerned with how to locate the needed data (registries), how to know the data history (metadata) and much more. It is stressed that XSAMS is not a system for storing data; XSAMS can be adopted for a database without changing the way data are stored, only changing the way in which they are communicated. It does constitute an important step beyond a multi-database search engine such as GENIE, which has to accept data in whatever format they are communicated by each covered database. It constitutes a very big step over old methods such as ALADDIN, which is based on 30-year-old technologies (Fortran-77) and relies on ASCII files of a rigid fixed format. Data exchange is presently spear-headed by emerging internet technologies (IT). Key words are structure, consistency and relationships.

XSAMS employs the eXtensible Markup Language (XML) that was developed to facilitate sharing of heterogeneous data across different systems, particularly systems connected to the internet. XML is a metalanguage, i.e., a tool for development of new languages, and XSAMS is such a new language. It clearly separates content from presentation and allows specification of constraints. For example, an atomic energy level might be presented in the form <energy units="eV">2.306</energy>, with the constraint that the content is a real number, and angular momentum might be presented in the form <total_J>1.5</total_J>; <total_L>1</total_L> with J restricted to be integer or half-odd integer and L restricted to be nonnegative integer. The goals of XSAMS are to develop a (rather) complete set of rules (XML tags, document structure, relations, etc.) for description of atomic and molecular, and later plasma-material interaction, data sets. In the XSAMS tree there are States (of atoms, molecules, solids and elementary particles), Processes (collisional, radiative, non-radiative), and Functions, Methods, and Sources. Already for atoms there is a significant hierarchical organization of the data, starting with the element, then the isotope, the charge state, the excited state, and finally the quantum numbers and the (configuration-interaction) composition of the state. The associated non-numerical data may include bibliographical information about the data provenance.

The present status of XSAMS is that it is publicly available with documentation at the IAEA web site, http://www-amdis.iaea.org/xsams/. Work continues on the introduction of new XSAMS elements and attributes and also new large sections, e.g. for describing a plasma environment or for describing atomic or molecular line broadening. The dedicated involvement of the VAMDC project is most important. Implementations are being carried out at different places and as a result there are ongoing discussions and ideas on improving the language.

Dr Marie-Lise Dubernet described the Virtual Atomic and Molecular Data Centre (VAMDC), http://www.vamdc.eu (.org). Background of the project is the interest in standards for data exchange. Discussions about interoperability of A+M data took place at an Atomic Data and Analysis Structure (ADAS) meeting in 2003, and then in September 2004 definition of standards started in two parallel efforts: work in the International Virtual Observatory Alliance (IVOA led to the Simple Line Access Protocol (SLAP) and the Simple Spectra Line Data Model (SSLDM), and work in collaboration among NIST, the IAEA, the Observatoire de Paris and ORNL led to XSAMS. SLAP and SSLDM are limited in scope relative to XSAMS, but they have already implemented tools; see http://www.ivoa.net/Documents. As an official project VAMDC started in July 2009, with substantial EU e-Infrastructure Program Project funding for a period of 42 months. There are 15 legal partners encompassing 21 institutes or departments from 6 EU countries, the Russian Federation, Venezuela and Serbia, and there are 2 external partners (NIST and CFA, Harvard). The project may live beyond the 42 months as a laboratory without walls.

The Challenge for VAMDC is to provide data access to all A+M data to all end user communities. The data underpins many areas of research, not limited to plasma- and astrophysics, and the potential users come from industry as well as academia. The data is complex and increasingly large, and the handling of the data often involves the use of application tools. There are issues with ensuring data completeness and quality. With all that in mind the key VAMDC objectives are: (1) to implement a VAMDC interface for accessing major existing databases containing heterogeneous data and aimed at different users; (2) to enable data queries across multiple databases each focused on specific research topics; (3) to facilitate the data publishing and quality control process for major A+M data producers; and (4) to involve wide user and producer communities in the development and use of VAMDC tools. The key end user communities are from astrophysical, atmospheric, plasma and combustion science and from the industrial applications field. They perform simulations, observations, and diagnostic interpretation. There is also a teaching outreach component to VAMDC. In the VAMDC infrastructure it is foreseen that the user accesses a database through some application that is also part of VAMDC. The application connects with the relevant databases and code services and communication takes place according to standardized formats agreed by VAMDC. In the VAMDC project there are networking activities (training and workshops; connections to other groups), service activities (deployment of A+M database and code services, support to the service and user communities) and research activities (standards development, e.g. XML Schema, dictionaries, a query language, a registry; and publishing and data mining tools).

Dr Dubernet emphasized that at this stage VAMDC is seriously interested in XSAMS, but is not committed to it. For spectral lines SLAP and SSLDM, developed in the framework of the IVOA, are alternatives. SLAP (http://www.ivoa.net/Documents/SLAP) defines a protocol for retrieving spectral lines from different spectral line databases through a uniform interface. The interface is meant to be reasonably simple to implement by service providers. A basic query will be done in a wavelength range for the different services. The service returns a list of spectral lines formatted as a VOTable. SSLDM (http://www.ivoa.net/Documents/SSLDM/) is integrated with SLAP to allow seamless access to spectral line transitions available worldwide. In SSLDM objects and attributes are defined to characterize properties of lines that are important in astrophysical contexts. SLAP and SSLDM could be a model for further more complicated applications to collisional data and then possibly molecules and surfaces.

For collisional data the Basecol database (http://basecol.obspm.fr) is an important target for XSAMS or for alternative access protocols. Basecol contains published excitation and de-excitation rate coefficients and level data, presently for 21 target molecules and for perturbers H, He, H_2 and e^-.

Basecol embodies a carefully annotated bibliographic database, calculated collisional rates, graphical visualization of collisional rates, fitted and analytic functions of the collisional rates and the associated coefficients, information on the methods used in the calculation of cross sections and rate coefficients, and energy levels of the molecules taken from spectroscopic databases or theoretical calculations. The rate coefficients tables are linked to tables containing the correspondence between labelling of states and their quantum numbers and energy levels. They are also linked to tables containing the corresponding fitted coefficients as well as the fitted functions. The format for data exchange is the VOTable (an example is shown in the talk), but also ASCII can be used. The Basecol, SLAP and SSLDM examples raise issues for VAMDC, many of which must be resolved within the next few months: Should we have general enough schemas or different schemas for different fields? Should we allow different data models and make conversion tools, or try to convince everybody to use a single data model? Can we use schemas for all A+M data? Can we use schemas for very large quantities of data? How complicated can we allow the registries and the query languages to be? How do we converge fast enough in order to produce something useful to users?

The VAMDC deliverables are organized in 8 Work Packages (see the link on the main VAMDC web page) and Dr Dubernet briefly reviewed the plans for the first year, Cycle 1, of the project. She highlighted the User Requirements questionnaire on the main web site, the development of publishing and standards policies (Dr Evelyne Roueff is in charge of this task), the Annual Meeting (April 19-22 at Milton Keynes, near London), the database implementation activities in WP4, the service and grid tool activities in WP5, the schema, dictionary, query language and registry activities in WP6, the conversion tools library activities in WP7 and the prototyping activities in WP8. The schema activities in WP6 and the prototyping in WP8 are of very much interest for the XSAMS project. It is intended to have substantial prototyping involving XSAMS done already in time for the annual meeting. There should be a prototype convertor for DB output to XSAMS, most likely for Basecol and for the Vienna Atomic Line Database (VALD). There should be a toolbox for converting between VOTables and XSAMS. There should be a prototype query conversion tool from generic SQL to, e.g., VALD requests. There should be prototype registry specifications for query/registry interaction. There should be a generic open source database equipped with tap interface generating XML output in response to an SQL query that is then converted to XSAMS. In other words, it is intended to prototype the entire sequence, SQL request → Database → Output → XML/VOTable → XSAMS, and (registry). To review the key dates in 2010 for VAMDC: following the annual meeting the Cycle 1 report is due in June and then also the plans for Cycle 2 must be specified. The first Strategic Advisory Board meeting will be held between June and October, and by 1st October the critical review of the level 1 VAMDC prototype for Cycle 1 will take place. Finally, negotiations are underway to add KAERI as a new partner in VAMDC.

Dr Yuri Ralchenko described the work at National Institute of Standards and Technology (NIST) on atomic databases and associated online tools. The most important numerical atomic database at NIST is the Atomic Spectra Database (ASD: http://www.nist.gov/physlab/data/asd.cfm). It contains critically evaluated NIST data for radiative transitions and energy levels in atoms and atomic ions. Data are included for observed transitions of 99 elements and energy levels of 57 elements. ASD contains data on about 950 spectra from about 0.4 Å to 500 μm, with about 77,000 energy levels and 144,000 lines, 60,000 of which have transition probabilities. Following general principles for databasing at NIST only published and evaluated data are included and accuracy must be reported. The data are consistent between spectral lines and atomic levels, which are both in the ASD. The database is built on MySQL RDBMS and the interface was developed at NIFS using Perl, Java and JavaScript. The interface offers some online derived data in addition to the static data. The database is heavily used; over 400,000 queries were made for spectral lines and over 135,000 for energy levels in the first 11 months of 2009. Compiling new data involves a critical evaluation of the literature, the assessment and possibly change of line identifications, the optimization of energy levels based on multiple sources, the assignment of accuracies, and an internal NIST quality review. A new compilation for Ti is almost finished, a new compilation for Ar is undergoing internal review, and work is in progress on Ba and Sr (many charge states), Ni I and II, and H, He, Li, Be, B, F, Ne and Ar I. Other compilations since 2006/2007 are concerned with Kr, Si, S, Na, Xe and Al (all many charge states) and with Hg I. A new version of ASD, v. 4.0, is currently being tested for intended

release in about 3 months. It contains more spectral lines and levels and is fully integrated with the bibliographical databases.

There are several bibliographical atomic databases at NIST; concerned with atomic energy levels and spectra, transition probabilities, line broadening, and energy levels and transition probabilities (integrated with ASD). The content has been enriched with direct HTML links to online papers through Digital Object Identifiers. The literature is searched automatically and updates are made on a daily basis. The number of records has grown from 20,000 in 2006 to about 30,000 now.

In addition to the Atomic Spectroscopy Database and the numerical databases the Physics Laboratory at NIST is involved in collisional radiative plasma modeling. Dr Ralchenko is principal convener of the NLTE (non-local thermodynamic equilibrium) series of workshops that meet every two years, most recently NLTE-6 in Dec 2009 in Athens, Greece. These are code-comparison workshops that each revolve around some well-defined test cases – a specified impurity in a well-defined plasma environment. The results of the workshops contribute to the NIST Saha Plasma Kinetics Modeling Database, which contains benchmark results for simulation of plasma population kinetics and emission spectra.

Dr Jun Yan presented work in the China Research Association of Atomic and Molecular Data (CRAAMD) collaboration. CRAAMD was initiated in 1987 with the objective to coordinate data compilation, evaluation and production. There are 10 active participating groups, listed here together with their principal contact person and area of interest. 1) Institute of Applied Physics and Computational Mathematics, Beijing, Yan Jun, theoretical calculation of atomic data and simulations of radiative properties of both LTE and non-LTE plasmas. 2) Institute of Modern Physics of the Chinese Academy of Sciences, Ma Xin-Wen, heavy particle collision experiments. 3) Graduate School of the Chinese Academy of Sciences, Qu Yi-Zhi, theoretical calculation of cross sections for heavy particle collision processes and data evaluation. 4) Fudan University, Chen Chong-Yang, electron-ion collision theory and experiment. 5) Sichuan University, An Zhu, measurements of atomic inner-shell ionization cross sections. 6) Jilin University, Ding Da-Jun, molecular spectra data compilation. 7) Science and Technology University of China, Zhu Lin-Fan, electron-atom and electron-molecule collision experiments. 8) National University of Defense Technology, Yuan Jian-Min, theoretical calculation of opacity of LTE plasmas based on DLA model. 9) Tsinghua University, Mo Yu-Xiang, ionization potential of molecule ions and vibrational and rotational resolved molecular spectra based on ZEKE facility. 10) Northwest Normal University, Dong Chen-Zhong, theoretical calculations of energy levels and radiative transition properties for M-shell Au ions.

The database work of CRAAMD is concentrated at the Atomic and Molecular Data Research Center in Beijing and is supported by the Institute of Applied Physics and Computational Mathematics (IAPCM) and by the Chinese National Committee for CODATA. The atomic and molecular databases may be accessed through http://www.camdb.ac.cn/e/. The atomic database includes information about ionization potentials, levels, spectra, electron-impact excitation, electron-impact ionization, dielectronic recombination, autoionization, photoionization and opacity, and it has a bibliographical component. Sections on heavy particle collisions and quantum defects are planned. The molecular database includes information about ion-molecule and electron-molecule collisions. A section on molecular spectroscopy is planned.

A set of generalized oscillator strength (GOS) and GOS density (GOSD) data for sodium was recommended by CRAAMD, which include the transition from the ground state [2p63s]3 2S excited to [2p6(n+1)s](n+1) 2S,[2p6np]n 2P,[2p6nd]n 2D ($3 \leq n \leq \infty$) and adjacent continuum states, as well as to some autoionization states. These data were calculated using modified R-matrix codes based on a set of elaborately optimized target orbital bases and were verified to be of high accuracy.

A large amount of data was produced by CRAAMD in past years. That brought forth an issue, which may be a general issue for data work, that it is almost impossible to evaluate all these data critically, especially the calculated data. (This also applies to on-line data calculations.) In principle, for sure, the recommended data should be reliable, like the NIST atomic spectroscopy data. On the other hand, these calculated data may provide a systemic collection consisting of energy levels and rate

coefficients of all dynamic transition processes and covering the ground and excited states of many ionic stages. Such data may be very much of interest to users in astrophysics or fusion sciences for applications in plasma simulation and plasma diagnostics, even though we know that those calculated data are not very precise; for example, errors may be 10% to 30% compared with the measurements, and the accuracy may be even poorer for weak transitions. Therefore, one hesitates to include these data into the database, and many of the data produced by CRAAMD have not been included in its database. At present the principle of CRAAMD for including newly produced data is (1) to include all the critically assessed data, and (2) to include systemically calculated data, which must be sampling evaluated and for which evaluation reports must be provided to help the user judge the quality.

Dr Yongjoo Rhee presented work on atomic spectroscopy and the atomic, molecular and optical (AMO) database (http://amods.kaeri.re.kr/) in the Laboratory for Quantum Optics at the Korea Atomic Energy Research Institute (KAERI). The Atomic Spectroscopy Research Group (ASRG) in the laboratory has an experimental program devoted to the precision measurement of atomic spectroscopic parameters such as energy levels, autoionization levels, isotope shifts, hyperfine structures, multi-photon ionization schemes, etc., using the resonance ionization spectroscopy methods. The ASRG is also responsible for the AMO database systems (AMODS). Supporting theoretical work at ASRG is concerned with relativistic electronic structure calculations, electron collision processes, and density-matrix based calculations. The research in the group is motivated by basic atomic physics and by applications to magnetic and inertial confinement fusion energy research, industrial plasmas and laboratory astrophysics.

Recently the ASRG has made many studies of lanthanide elements, particularly La, Sm, Eu, Gd, Dy, Er and Yb. Isotope shifts were measured in transition lines in neutral Sm and were compared with single-configuration and multi-configuration Dirac-Fock calculations. Isotope shifts and hyperfine structure were also studied in neutral Yb. The MCDF code due to Desclaux, Indelicato and Kim, is used for the calculations and an interface to this code is available through the AMODS web service. The laboratory has also studied and modelled spectra of highly charged heavy ions such as W, Mo and V. Tungsten (W) is of particular interest for fusion as the primary plasma-facing material in ITER. The MCDF code has been used to calculate emission lines and line shapes for highly charged W ions. Spectra were calculated for W^{33+} to W^{46+}.

In addition to spectra, electron impact ionization cross sections are essential data for fusion plasma and can be calculated by using MCDF code. The calculations rely on the Binary Encounter Bethe (BEB) model and employ the plane wave Born (PWB) approximation for a neutral atom and the Coulomb Born (CB) approximation for a singly charged ion. Electron impact ionization cross sections of neutral atoms are very difficult to obtain experimentally; however, W, Mo, V, Li, Be, C and others have been studied in the ASRG recently. Also electron impact ionization cross sections of W^{+} have been calculated and compared with experiments. Electron impact ionization cross sections of neutral W atom have been calculated at ASRG and compared with other calculations. AMODS now offers an interface that permits online calculation of direct ionization cross section bases on BEB for W and Mo.

The AMODS database contains information on atomic and molecular structures, transition lines and probabilities, laser propagation characteristics, collisional ionization cross sections, and fundamental constants. Dr Rhee showed the interface in his presentation. Spectral lines can be searched per atom or ion with or without specification of the precise charge state, and the information is connected to bibliographical data. Computational tools are provided that interact with the database to obtain population dynamics and to calculate the deposited power of a laser beam. Total and differential electron impact excitation and ionization cross-sections are available in AMODS for several target atoms and molecules; see http://amods.kaeri.re.kr/impact/IMPACT.html. Both theoretical and experimental data are included. In collaboration with NIFS data for autoionizing states and dielectronic satellite lines are being assembled into AMODS.

In conclusion, the Atomic Spectroscopy Research Group at KAERI is a unique atomic spectroscopy facility in KOREA in which experiments and theoretical studies are being pursued. Recent spectroscopic studies for fusion research have addressed electron impact ionization cross sections

(W, Mo, Be, C, etc) as well as radiative transitions of highly charged ions and of moderately charged W ions. The BEB model was extended to higher charged states and the MCDF code was upgraded. High energy density science for inertial fusion and laboratory astrophysics is another concern and the ASRG has been involved in the production of data (EOS, opacity) and in simulation (HYADES, MULTI). Computer codes for fusion plasma are under development, including codes for non-LTE plasma and for a two-temperature model.

Dr Bas Braams described the work in the IAEA Atomic and Molecular Data Unit; see http://www-amdis.iaea.org. The Coordinated Research Project (CRP) is the principal mechanism that the Unit has to encourage scientific research. In a CRP up to approximately 15 institutes from around the world are represented. The CRP runs for 3-4 years, with research coordination meetings at approximately 1.5-year intervals and usually held at IAEA Headquarters. The IAEA supports attendance at the research coordination meetings, but has only very small funds for direct research support. The CRPs of the unit are focused on A+M and Plasma-Material Interaction (PMI) data for fusion. A final report is prepared for the IAEA journal "Atomic and Plasma-Material Interaction Data for Fusion", and data produced in the course of the CRP are normally included in the ALADDIN database. Information about ongoing and recent CRPs is collected at http://www-amdis.iaea.org/CRP. Recent CRPs are: "Atomic Data for Heavy Element Impurities in Fusion Reactors" (2005-2009), which focused on atomic processes for noble gases Ar, Kr and Xe, likely wall material W, and other possible impurities Fe, Cl and S; "Data for surface composition dynamics relevant to erosion processes" (2006-2010), which is especially concerned with migration processes in a C-Be-W mixed wall and also with surface processes of B, Mo, Ti and other elements; "Characterization of Size, Composition and Origins of Dust in Fusion Devices" (2008-2012), concerned also with dust removal techniques and impact of dust on tritium retention; "Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions" (2009-2013), concerned with atomic and molecular processes involving H, He, Li, Be, B, C, N, O and their hydrides in edge and divertor plasma; and most recently "Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV" (2010-2014). The tungsten CRP has been approved and proposals for participation are now being solicited. The CRP will focus on radiative and collisional processes for W ions in fusion plasma, including excitation and ionization by electron, photon, and proton impact, auto-ionization, radiative de-excitation and recombination, dielectronic recombination, and charge exchange, and in all cases looking for cross-sections as well as spectroscopic signatures, based on experiment and theory. Meetings will likely be held in Q4 2010, Q2 2012 and Q4 2013.

The A+M Data Unit maintains its AMBDAS bibliographical database, which goes back to the 1970s and is based on primary compilations done at ORNL and NIST. (Other institutions have contributed, but not in the most recent years). In 2010 there are about 50,000 entries in AMBDAS. An affiliate agreement has recently been made with CrossRef, manager of the DOI registry, to get access to their data so that a doi-link can be made part of the AMBDAS query response. The A+M Unit also maintains the ALADDIN numerical database for A+M collisions and plasma-material interactions. This database goes back to original work by Yuri Ralchenko for A+M data; the interface was revised by Yuri Ralchenko and Predrag Krstic in 2005 and an interface for plasma-material interaction data was added by Predrag Krstic, Fred Meyer and Denis Humbert in 2007. The contents are largely based on IAEA Coordinated Research Projects. The data are expected to be the best available ones at the time that they are first entered into the database, but the coverage is not at all comprehensive and older data may not be the best that is available at present. In order to provide convenient access to many numerical databases the A+M Unit maintains the GENIE search engine, which is also original work of Yuri Ralchenko. It provides access at this time to 8 databases for radiative properties and 4 databases for electron-impact collisional processes. It is of interest to extend GENIE to access further databases, also including heavy particle collisions and molecular processes, and bibliographical data. In new work, mainly by Hyun Chung, the A+M Unit is developing a Wiki-style Knowledge Base for atomic, molecular and plasma-material interaction data and their context in fusion, astrophysics, spectroscopy and elsewhere. At present the basic layout is being developed, and it can be seen at http://www-amdis.iaea.org/w. The wiki will not be completely open to outside contributors, but the intent is to engage many, including anyone who is known from the A+M Unit activities, and their colleagues too. To conclude the presentation on activities of the A+M Unit the Data Centre Network

(http://www-amdis.iaea.org/DCN) and Code Centre Network (http://www-amdis.iaea.org/CCN) were briefly described.

3. Discussion and Work Plan

The more technical discussions were led off by a review from Dr Marie-Lise Dubernet of an evaluation of XSAMS that is taking place within VAMDC. VAMDC is committed to XML-based standardization of means of communicating atomic and molecular data, but they are not committed to using XSAMS for that purpose. The issue will be an important topic of discussion at the VAMDC annual meeting, 19-22 April, and it should be resolved by this summer. For VAMDC the choice is between on one hand XSAMS as a comprehensive approach and on the other hand an approach that they call "case-by-case". In the case-by-case approach appropriate XML tags are selected for each particular database. The case-by-case XML structure would be much flatter than XSAMS, which has a deep hierarchy. A mapping from "case-by-case" to XSAMS could be done on an ad-hoc basis if it is needed.

Criticisms of XSAMS that "case-by-case" is meant to address include that it is too verbose, too complex, the hierarchy leads to very deeply nested XML, some quantities are not used systematically, it is said to be hard to extend XSAMS to new cases and to deal with unusual quantum numbers and symmetries. These criticisms (neutrally reported by Dr Dubernet) raised plenty of discussion. Participants agreed that XSAMS is more complicated and has a much deeper hierarchy than would be needed in an XML Schema that is designed for any single database. On the other hand, in the discussions it was stressed that XSAMS is not meant as a means of storing data, only as a means of communicating the data. If it is intended to facilitate the communication of data from one A+M database to another then one has to anticipate all kinds of physical properties that might be used as tags or descriptors in such a database, and one is pushed in the direction of XSAMS. (Later in the meeting, see below, Drs Loboda, Gagarin and Ralchenko demonstrated transmission of data from the NIST Atomic Spectra Database through XSAMS to the VNIITF Spectr-W^3 database.)

In the ensuing discussion about the complexity of XSAMS and the difficulty of extending it to new cases it was stressed that such extensions should almost always be backward compatible, as is achieved by making the new tags optional. New cases aren't going to arise very often; however, there are areas in XSAMS that will need further development. The description of molecular vibrational states was mentioned as an important example where further development is needed. Rotational states are probably well described, but the interaction between rotational and vibrational descriptors at high excitation level is a very difficult problem. As an example of the verbosity of XSAMS the description of a state of ammonia was discussed. In any case it is important to provide with XSAMS some sort of "case-by-case" documentation, showing how it is employed for the most common applications.

Still loosely coupled to the evaluation of XSAMS by VAMDC the discussion then turned to the treatment in XSAMS of line broadening and line shifting. At present this is not handled by XSAMS, because it isn't a pure atomic property, it depends on interaction with the environment. How to incorporate plasma parameters into XSAMS was the subject of much discussion later in the meeting (see below).

The VAMDC researchers are very much interested in molecular data and there are several issues that need further attention. Properties are not yet included: at this time XSAMS does not offer a way to specify a dipole moment or a polarizability. It is not possible to identify individual atoms in molecules, and this is important for describing isotopic substitutions or couplings to nuclear spin. The structure of the description of rotational and vibrational states raises questions; why is this included as part of the electronic state, and how can it handle the coupling among the two at large vibrational energies? Quantum numbers occur perhaps in too many different places in the XSAMS tree. The description of chemical species needs to be improved, and in particular it needs to be seen if somehow the Chemical Markup Language (CML) can have a role in XSAMS. Also it is important to check and review all the constraints that may be valid for quantum numbers and other parameters.

The technical discussion continued with a presentation by Dr Peter Loboda and Dr Sergey Gagarin on issues found in their work at Zababakhin on the Spectr-W^3 database, http://spectr-w3.snz.ru/. The Ritz-value is repeated in several places in the hierarchy and it is suggested that the EnergyWavelengthType could be simplified. This raised discussion; the simplification wasn't completely obvious and it was urged that proposed changes should have a trial implementation in the schema to see all the places that are affected. A second issue concerns the Radiative Transition Type. There is interest in radiative transitions of which the description involves bundled atomic states, or super-configurations, and the schema needs further development for that purpose. Closely related to this are issues concerning satellite line data and satellite branching ratios and intensity factors; such data could be made part of the Radiative Transition Type. A further issue with these data is the need for a label to characterize soft X-ray lines. A field Radiative Transition Label is proposed.

There were other issued found in the work on Spectr-W^3. In the Nonradiative Transition Type there is a mandatory parameter Probability; it is suggested to make it optional. In the Atomic Numerical Data Type there is a need for new optional elements Total Radiative Lifetime and Total Nonradiative Lifetime.

Dr Akira Sasaki reported on his use of XML to define atomic levels. This work was done independent of XSAMS, but the experience is of interest anyway. He considered the description of atomic levels to see how an XML based format may be useful for performing plasma modeling. Scientists regularly abbreviate complex atomic level descriptions; for example writing "4p 5", omitting closed shells, or writing "1s nl" for a group of levels. Checking the range of quantum numbers and occupation numbers is useful for finding erroneous expression such as "1p" or "1s 3". Functions for handling such expressions and for validation and testing can be included in XSAMS, but it may be easier to use a post-parser, based on simple language processing techniques using regular expressions. The post-parser would also be useful for visualization of data, which will help with human checks of the encoding; it improves the user interface and promotes the reliability of the data. Such a post-parser could perhaps be added to an XSAMS-based system as well.

Mr Denis Humbert reported on technical aspects of database work at NIFS. There are many databases at NIFS that could benefit from XSAMS, also for particle-surface interactions, although the initial focus should be on electron-atom collisions. NIFS provides also fit functions for many cross-sections, and it would be of much interest to incorporate such fit functions into XSAMS. Until now there has been no feedback on that option. The principal database, AMDIS, is under migration this year and that provides a good motivation to develop a new web interface. XSAMS is being considered in that role, but it will probably take beyond the year 2010 for results to be available. Some trial specifications for use of XSAMS with AMDIS are being developed.

The technical discussions continued on Friday, starting with a review by Dr Yuri Ralchenko of issues concerning atomic data (not molecules, not surfaces). An issue had been raised about how to use XSAMS for search of atomic data and the reply is that XSAMS isn't meant for search; it is meant for robust transmission of data. There was a request to add 1/m as a unit for wavelength in addition to 1/cm (and other units, such as eV), but this was held to be not important. There is a request for quadrupole and higher order transitions, presently not described in XSAMS, and Dr Ralchenko recommends that they be included. There is a request for including new designations for atomic configurations. The most important request is for a description of spectral line shape and line broadening due to interaction with the plasma environment and this was the subject of much discussion. Participants reviewed and compared two possible treatments of this interaction. In one treatment one takes the point of view that the principal environmental parameter is the electron temperature, and then the basic data type for line-width is that of a one-dimensional table with T_e as the independent variable and line width as the dependent one; this is similar to treating a cross-section as a function of collision energy. In the other treatment one takes the point of view that the environment is in principle much more complicated than just electron temperature; plasma composition can be important, and the separate electron and ion temperatures, and one should use a general data type that is the environment, and then with each particular numerical line-width entry there is a pointer to an instance of the environment data type. The general sentiment at the meeting

was first that line-width is important and needs to be handled by XSAMS, and second that probably it should be done via a new generic data type for environment. However, this needs to be prototyped. Somewhat on the side of this discussion it is noted that similar issues apply to the description of plasma-material interaction, now with surface temperature as an environmental parameter. In that case too one has the option to represent, say, a reflection coefficient as a one-dimensional array with surface temperature as independent variable, or alternatively to introduce a new data type for "surface condition", which then includes temperature as one of its fields.

At this point a demonstration was made of the value of XSAMS for transmitting data; the result of an exercise initiated the previous afternoon between Dr Ralchenko, Dr Loboda and Dr Gagarin. In the prototyping work at VNIITF Dr Gagarin had developed code to take spectroscopic data in XSAMS format and convert it to the internal Spectr-W^3 database format. In the prototyping work at NIST Dr Ralchenko had developed code to write an ASD query response in XSAMS format. A sample record from ASD extracted by Dr Ralchenko's prototype was passed via XSAMS to Dr Gagarin's code and was successfully read into Spectr-W^3.

As the meeting neared its close the issue of plasma-material interaction was briefly noted, but participants agreed that at this time it is appropriate to concentrate on atomic and molecular issues in the further development of XSAMS. Perhaps at the next meeting it will be possible to see some early use of XAMS for surface data.

4. Conclusions

Interest in XSAMS is strong as was shown by the presence at this meeting of participants from several atomic and molecular data centers and research groups from Japan and neighbouring countries. The work on XSAMS in the European Virtual Atomic and Molecular Data Centre (VAMDC) is very important for the future status of the Schema and participants in the meeting look forward to the results of their prototyping exercises and the further evaluation of the use of XSAMS in VAMDC. The initial implementation of XSAMS on the Spectr-W^3 database at VNIITF and the demonstration of communication through XSAMS with the NIST Atomic Spectra Database are very encouraging. Some general scientific issues for the further development of XSAMS are the treatment of the plasma environment and of spectral line shifts and line broadening in the atomic data section, and for molecular data the treatment of coupled rovibrational states at high excitation, the inclusion of properties other than energy, and of properties of atoms within molecules. The nearest event for further presentation and discussion of XSAMS is the VAMDC annual meeting 19-22 April, and following that the EGAS/ECAMP meeting 5-9 July and the ICAMDATA meeting 21-24 September.

Appendix 1

IAEA Consultants' Meeting on XSAMS: XML Schema for Atoms, Molecules and Solids

24-26 March 2010, National Institute for Fusion Science, Toki-City, Japan

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Appendix 2

IAEA Consultants' Meeting on XSAMS: XML Schema for Atoms, Molecules and Solids

24-26 March 2010, National Institute for Fusion Science, Toki-City, Japan

AGENDA

Wednesday 24 March, morning **Building: A1 – Room: A402**

09:00 – 10:15 Guided tour of Large Helical Device (LHD) experiment

10:30 – 11:30 Show of the CompleXcope visualization facility

11:30 – 13:30 *Lunch*

Wednesday afternoon **Building: A1 – Room: A402**

13:30 – 13:50 Opening remarks and Welcome, Professor Motoyasu Sato, Director of the Coordination Research Center, and Izumi Murakami

13:50 – 14:00 Last meeting minutes review and adoption of the agenda, Bas Braams

14:00 – 14:30 Database work at NIFS, Izumi Murakami

14:30 – 15:00 Work of the ICSU Strategic Coordinating Committee on Information and Data (SCCID), Professor Masatoshi Ohishi from National Astronomical Observatory and Japanese Virtual Observatory

15:00 – 15:30 *Coffee/Tea break*

15:30 – 15:55 Database activities at Observatoire de Paris-Meudon, Evelyne Roueff

15:55 – 16:20 Database activities at RF Nuclear Center Zababakhin, Peter Loboda

16:20 – 16:45 Database activities at Korean National Fusion Research Institute, Jung-Sik Yoon

16:45 – 17:15 Introduction to XSAMS, Yuri Ralchenko

Wednesday Evening *Dinner in Tajimi*

Thursday 25 March, morning **Building: A1 – Room: A402**

09:00 – 10:00 Database activities at VAMDC, Marie-Lise Dubernet

10:00 – 10:30 Database activities at NIST, Yuri Ralchenko

10:30 – 11:00 Database activities at CRAAMD/IAPCM, Jun Yan

11:00 – 11:30 Database activities at Korea Atomic Energy Research Institute, Yongjoo Rhee

11:30 – 12:00 Database activities at the IAEA, Bas Braams

12:00 – 13:30 *Lunch*

Thursday afternoon **Building: A1 – Room: A402**

After lunch we move into the more technical phase of the meeting, focussed on XSAMS. In the agenda at most times someone has the floor, but the speaker is primarily introducing issues for discussion and the presentation and the discussion will be inter-mingled.

13:30 – 14:30 XSAMS evaluation by VAMDC, Marie-Lise Dubernet

14:30 – 15:00 XSAMS issues found at Zababakhin, Peter Loboda and Sergey Gagarin

15:00 – 15:30 *Coffee/Tea break*

15:30 – 15:50 Experience with XML for atomic levels, Akira Sasaki

15:50 – 16:20 XSAMS issues found at NIFS, Denis Humbert

16:20 – 17:15 Continued discussion on A+M issues in XSAMS

Thursday Evening *Dinner in Tajimi*

Friday 26 March, morning **Building: A1 – Room: A402**

09:00 – 10:30 Further discussion of atomic data issues, led by Yuri Ralchenko

10:30 – 11:00 *Coffee/Tea break*

11:00 – 12:15 Web and documentation issues

12:15 – *Meeting closed*

12:15 – 13:30 *Lunch*

Friday afternoon **Building: A1 – Room: A402**

13:30 – 15:00 Available for continued technical collaborations

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