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XML Schema for Atoms, Molecules and Solids (XSAMS)

Summary Report of an IAEA Consultants' Meeting

Campus of the University of Vienna

Vienna, Austria

20-22 February 2012

Prepared by

B. J. Braams

December 2013

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Abstract

A Consultants' Meeting on "XML Schema for Atoms, Molecules and Solids (XSAMS)" was held in conjunction with the Virtual Atomic and Molecular Data Centre (VAMDC) Cycle Three Project Meeting on the Campus of the University of Vienna on 20-22 February 2012. The meeting was to agree on the adoption of an international standard XSAMS version 1.0 and to discuss implementation activities and user experience with the schema. The proceedings of the meeting are summarized here.

December 2013

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1. Introduction

The XML Schema for Atoms, Molecules and Solids (XSAMS; see http://www-amdis.iaea.org/xsams/) is a developing standard for exchange of atomic and molecular data. An initial release was made in 2009 under IAEA responsibility. XSAMS was adopted by the Virtual Atomic and Molecular Data Centre (VAMDC; see http://www.vamdc.org), an EU Framework-7 project, as their standard for data exchange and implementations commenced on all databases represented in VAMDC. From that time on development of XSAMS was driven by the needs of VAMDC.

VAMDC held its 3rd annual project meeting in Vienna on Tue-Fri 21-24 February 2012 and it was decided to use the opportunity to organize a Consultancy Meeting on XSAMS on the overlapping days Mon-Wed 20-22 February 2012, with the primary objectives to review XSAMS developments, agree on an international standard XSAMS version 1.0, and review future maintenance of the Schema.

Participants in the meeting were generally deeply involved in the VAMDC project as well. Therefore the discussions at the XSAMS meeting were at the same time contributing to the development of VAMDC XSAMS version 1.0, the final XSAMS version of the Framework-7 VAMDC project.

The meeting was hosted by the Mathematics department of the University of Vienna and held on the main campus of the university with local organizer Prof Friedrich Kupka. On Monday the meeting was entirely devoted to XSAMS, on Tuesday and Wednesday it merged into the VAMDC meeting with broader and discussions of their atomic and molecular databases, and at the end of Wednesday an executive session was held to conclude the XSAMS part of the meeting.

Section 2 provides an Executive Summary of the Consultants' Meeting. Section 3 contains the meeting proceedings and Section 4 summarizes the conclusions. Appendix 1 contains the list of participants and Appendix 2 contains the meeting agenda.

2. Executive Summary

The Consultants' meeting on the XML Schema for Atoms, Molecules and Solids (XSAMS) was held in conjunction with the 3rd annual meeting of the VAMDC project, which relies on XSAMS and which has made many developments to the Schema. The objective of the meeting was to review the latest developments of XSAMS, to agree on the adoption of an international XSAMS standard and to discuss future development and maintenance of the Schema.

Participants strongly endorsed the developments made by the VAMDC project to XSAMS, both for atoms and for molecules. There is still some development going on before the expected end of project release of VAMDC XSAMS. In that light the meeting agreed as follows.

1. At this time VAMDC XSAMS matches the goals of IAEA XSAM and there should be a single XSAMS standard adopted by VAMDC and by IAEA.

2. The final version of VAMDC XSAMS (version 1.0, due in summer 2012) is to be adopted as the international standard XSAMS version 1.0.

3. IAEA must be prepared to take over maintenance of XSAMS following conclusion of the VAMDC project at the end of 2012. Procedures are to be discussed in the context of a possible long-term successor to VAMDC.

The defining documents for the agreed VAMDC XSAMS version 1.0 and International (IAEA) XSAMS version 1.0 is maintained at the VAMDC web pages under Standards: See the XSAMS 1.0 reference guide on the page http://www.vamdc.eu/documents/standards/.

3. Meeting Proceedings

Opening

The meeting was opened by Professor F. Kupka, local organizer for the overlapping XSAMS and VAMDC meetings, who welcomed participants to the Campus of the University of Vienna. It had originally been expected that on Monday (which was fully devoted to XSAMS) the meeting would be small, but there were already more than 30 people present. B. Braams extended his welcome and thanked the many additional participants for joining the meeting.

Presentations

M.-L. Dubernet: Overview of VAMDC XSAMS experience

Dr Dubernet provided an overview of VAMDC and the experience with XSAMS. Very briefly we recall here the VAMDC parameters: It is an EU Framework-7 infrastructure project from July 2009 to December 2012 having 21 partners, 3 non-EU external partners, 1 associated partner (IAEA), and providing a shared infrastructure for at this time 19 databases in the area of atomic and molecular spectroscopy and collisions, primarily focussed on the needs of plasma and astrophysics, but also looking at atmospheric science, plasma technology, lighting, fusion energy science and radiation science. These databases were entirely heterogeneous and the challenge for VAMDC has been to make them interoperable and connected. The project brings together different fields of producers of atomic and molecular data, it brings together data producers and data consumers and it provides connections among different research infrastructures such as Euro-VO, Europlanet and HELIO. The main technological centers for VAMDC node software, portal and standards development are at the Paris Observatory, the Cambridge Institute of Astronomy, Uppsala University and University College London with the Mullard Space Science Laboratory.

VAMDC has produced a major coherent body of standards for interoperability of their databases. XSAMS is the XML core for data communication, but there is also a query language, data access protocols, dictionaries and a registry, all documented on the VAMDC Standards web page.

Following these standards the project has developed a powerful web portal and desktop database access software to download and visualize data. The web portal can access VAMDC whole and discover data or selected databases can be accessed through the same interface. The project provides for technical support and training to users, maintenance and monitoring of the infrastructure, data preservation, quality assurance (of the infrastructure) and testing of database availability.

The project has extended XSAMS in multiple areas including description of molecular states (the "case-by-case" approach), line shapes, and solid spectroscopy. These developments were made independent of IAEA XSAMS and at a faster pace according to the needs of VAMDC. However, the IAEA XSAMS working group may decide to adopt and synchronize with VAMDC XSAMS in whole or in part.

VAMDC continues to develop new tools. On example is highlighted, the SPECTCOL tool to match spectroscopic and collisional data from different databases. The spectroscopic data include species, energies, frequencies, Einstein coefficients and (bibliographical) sources while the collisional data include species, energies (but different energies than in the spectroscopic DB), and rate coefficients. A major concern for the remainder of the VAMDC Framework-7 project period is to create a sustainable organizational infrastructure.

Yu. Ralchenko: Atoms in XSAMS

At the outset Dr Ralchenko emphasized that he is very pleased with the development of XSAMS within VAMDC. He then provided a brief overview of atomic data in XSAMS and raised some technical issues. The InChiKey is supposed to be unique, but an empty entry is allowed. The Accuracy field needs some attention, it is different in different places. Both for the Accuracy and for the Evaluation field clarification is needed on the meanings of various values and components. For nonradiative transitions the Width field needs to be described. The concept of Satellite Line should be made more precise. There are some minor issues with the treatment of environment, e.g. use of concentrations under Compositions and number densities under Environment. It is time to do something about the treatment of Units, which is really quite ad-hoc.

Ch. Hill: Proposed developments of the Molecules part of XSAMS

The molecules part of XSAMS is where the most substantial changes have been made by VAMDC since the release of XSAMS version 0.1 in 2009. Largely these changes are described by the catch phrase "case by case", referring to separate treatments of molecular states for each of (at present) 14 different molecular symmetries: general (gen), diatomic closed shell (dcs), Hund's case (a) diatomics (hunda), Hund's case (b) diatomics (hundb), closed-shell linear triatomics (ltcs), closed-shell non-linear triatomics (nltcs), closed-shell symmetric top molecules (stcs), closed-shell linear polyatomics (lpcs), closed-shell asymmetric top molecules (asymcs), open-shell asymmetric top molecules (asymos), closed-shell spherical top molecules (sphcs), open-shell spherical top molecules (sphos), open-shell linear triatomics (ltos), open-shell linear polyatomics (lpos) and open-shell non-linear triatomics (nltos). VAMDC has defined an individual set of quantum numbers and symmetries to describe data for each of these cases.

The case-by-case approach is largely settled now, but Dr Hill described other issues that are to be finally resolved for the next version of the Schema. For Functions in XSAMS it often makes sense to distinguish between "arguments," which have a clear physical meaning, and "parameters", which are usually associated with mathematical fit functions. This distinction is carried through in new objects DataType and DataFuncType. Various technical changes were made as well to VectorType, MatrixType and DataSeries.

In the area of line shapes, absorption cross sections and description of the environment there have been many developments made for VAMDC XSAMS since the original (2009) XSAMS version 0.1 release. Recent changes affect the description of collision-induced absorption cross sections, which is needed for the Hitran database. The description of transitions has been extended with a new TransitionKind element that incorporates besides electric and magnetic multipole transitions also polarization-related (Raman) transitions. Finally the treatment of accuracies and classification of evaluated data has been simplified.

Please see the Changelog in the VAMDC-XSAMS Reference Guide for more details on these changes.

N. Piskunov: User experience

Dr Piskunov described the experience of users (broadly defined) of VAMDC and XSAMS. In the course of its implementations XSAMS has already had a very positive influence on data providers. The Schema and VAMDC are designed for interoperability and this makes it natural to compare data from different sources. XSAMS demands full documentation of each data entry and thereby it flags

data incompleteness and hidden assumptions. Nearly all participating databases have found that implementation of XSAMS revealed problems in their data.

At the level of the "end user", the plasma or astrophysics scientist, XSAMS has not yet had much influence, but the latest VAMDC portal looks very attractive. The common interface to many databases is unique. The reasons for which XSAMS is valuable to database maintainers are also important to data users and it validates the choice to build the VAMDC infrastructure and use XSAMS for exchange of atomic and molecular data.

Dr Piskunov discussed future organizational and technical needs for VAMDC and XSAMS. In the near term the organizational needs are largely met by a hoped-for continuation of VAMDC beyond 2012 towards a sustained infrastructure. Among the technical issues there is work to be done still on a flexible XSAMS interpreter and tools to flatten XSAMS output into (cross-linked) tables as convenient input for existing codes.

XSAMS was an ambitious project and we should be clear about its limitations. It will not, for the foreseeable future, have a good description of solids. The description of molecules will be limited to the needs of the databases in VAMDC, so prejudiced towards small molecule spectroscopy more than chemistry. It is likely that more cases will be added in the future, but we don't expect a complete treatment of molecular processes. The treatment of atoms is reasonably complete, both for structure and spectra and for electron collisions.

Dr Piskunov made recommendations for future actions. The IAEA should take over the XSAMS standard, probably as developed by VAMDC at this time, and take responsibility for future maintenance of the standard. This responsibility includes to provide a home for bug reporting, development requests, and release of new versions. It needs to be done in close collaboration with the VAMDC successor organization. Following the completion of the VAMDC-XSAMS standard the documentation and relevant software should be transferred to IAEA, with the division of responsibility to be worked out as it becomes more clear how VAMDC will be sustained. Dr Piskunov recommends that there needs to be a workshop some time that brings together the VAMDC and IAEA XSAMS working groups and that sets up the procedures and infrastructure (version control system, bug and suggestions tracking system) for future development of XSAMS.

Discussion

Several broad issues came up in the discussions. The topic of units is treated in an ad-hoc manner in present XSAMS; they are defined as needed. So XSAMS has units cm5 (cm^5) that are used in the Hitran database for the collision induced absorption cross section, but it doesn't have cm6 or m5. It was discussed if the UnitsML Schema should be adopted as part of XSAMS, but participants agree that at present the ad-hoc approach is preferred.

Within VAMDC there are applications beyond the present range of XSAMS, notably to solid spectroscopy and to treatment of large molecules (PAH: polycyclic aromatic hydrocarbons). At this time the considered extensions in that direction are very modest; basically some keywords to describe solids. Some databases in VAMDC provide data on chemical reactions. Chemical reactions are in principle within the domain of XSAMS, but the existing XSAMS process codes are too limited especially in connection with three-body reactions.

Electronic molecular states are not well described by XSAMS. For atomic states there is also a fundamental issues with states that are described strictly numerically by an approximate full-CI

expansion without any particular assignment. It is agreed that these are limitations and one lives with them. The (pragmatic) philosophy is that expansion of XSAMS is driven by the needs of participating databases without asking for a comprehensive description of atomic and molecular processes.

Participants in the discussion all emphasized their general agreement with the developments made by the VAMDC project to XSAMS, for atoms and for molecules. For the present needs of VAMDC there are only rather minor issues that need to be resolved and VAMDC intends to produce its final XSAMS standard, VAMDC XSAMS version 1.0, by July or August 2012.

4. Conclusion

The following conclusions were reached.

1. At this time VAMDC XSAMS matches the goals of IAEA XSAM and there should be a single XSAMS standard adopted by VAMDC and by IAEA.

2. The final version of VAMDC XSAMS (version 1.0, due in summer 2012) is to be adopted as the international standard XSAMS version 1.0.

3. IAEA must be prepared to take over maintenance of XSAMS following conclusion of the VAMDC project at the end of 2012. Procedures are to be discussed in the context of a possible long-term successor to VAMDC.

Appendix 1

List of Participants

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Appendix 2

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

Campus of the University of Vienna

20–22 February 2012, Campus of the University of Vienna, Vienna, Austria

Scientific Secretary: Mr Bastian Braams

Agenda

Monday, 20 February 2012

10:00-10:30	Bastiaan Braams, Friedrich Kupka: Welcome and introductions
10:30-11:00	Marie-Lise Dubernet: Overview of VAMDC XSAMS experience
11:00-12:00	Yuri Ralchenko: Atoms in XSAMS
12:00-12:45	Christian Hill: Proposed developments of the Molecules part of XSAMS

Lunch

14:00-14:45	Nikolai Piskunov: User experience
14:45-17:00	All: Systematic review of the schema and agreeing on items

Agenda *(continuation…)*

Tuesday, 21 February 2012

10:00-17:30 Devoted to VAMDC Work Package (WP) and Node (participating project) reports.

Wednesday, 22 February 2012

09:00-17:00 Devoted to VAMDC Node reports and VAMDC Standards. This includes presentations and discussions led by Ch. Hill on XSAMS Standards and by A. Akram (with G. Rixon) on XSAMS tools.

17:00-18:00 XSAMS Steering Group meeting.

18:00 ***Close of XSAMS meeting***

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