

VAMDC

Virtual Atomic and Molecular Data Centre

**D4.5**

-

**Final Infrastructure Deployment Report**

Version 1.0

Grant agreement no: 239108

Combination of Collaborative Projects & Coordination and Support Actions



### **Project Information**

Project acronym: VAMDC  
 Project full title: Virtual Atomic and Molecular Data Centre  
 Grant agreement no.: 239108  
 Funding scheme: Combination of Collaborative Projects & Coordination and Support Actions  
 Project start date: 01/07/2009  
 Project duration: 42 months  
 Call topic: INFRA-2008-1.2.2 Scientific Data Infrastructure  
 Project web sites: <http://www.vamdc.eu>

<http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/WebHome>

### **Consortium:**

<b>Beneficiary Number *</b>	<b>Beneficiary name</b>	<b>Beneficiary short name</b>	<b>Country</b>	<b>Date enter project**</b>	<b>Date exit project**</b>
1(coordinator)	Centre National de la Recherche Scientifique	CNRS	France	Month 1	Month 42
2	The Chancellor, Masters and Scholars of the University of Cambridge	CMSUC	UK	Month 1	Month 42
3	University College London	UCL	UK	Month 1	Month 42
4	Open University	OU	UK	Month 1	Month 42
5	Universitaet Wien	UNIVIE	Austria	Month 1	Month 42
6	Uppsala Universitet	UU	Sweden	Month 1	Month 42
7	Universitaet zu Koeln	KOLN	Germany	Month 1	Month 42
8	Istituto Nazionale di Astrofisica	INAF	Italy	Month 1	Month 42
9	Queen's University Belfast	QUB	UK	Month 1	Month 42
10	Astronomska opservatorija	AOB	Serbia	Month 1	Month 42
11	Institute for Spectroscopy RAS	ISLAN	Russian Federation	Month 1	Month 42
12	Russian Federal Nuclear Centre All-Russian Institute of Technical Physics	RFNC-VNIITF	Russian Federation	Month 1	Month 42
13	Institute of Atmospheric Optics	IAO	Russian Federation	Month 1	Month 42
14	Corporacion Parque Tecnologico de Merida	CTPM	Venezuela	Month 1	Month 42
15	Institute of Astronomy of the Russian Academy of Sciences	INASAN	Russian Federation	Month 1	Month 42



This project is funded under “*Combination of Collaborative Projects and Coordination and Support Actions*” Funding Scheme of The Seventh Framework Program of the European Union

## **Document**

Deliverable number: D4.5  
Deliverable title: Final Infrastructure Deployment Report  
Due date of deliverable: December 2012  
Actual submission date: January 2013  
Authors: G. Rixon and WP4 team  
Work Package no.: WP4-SA1  
Work Package title: Infrastructure Deployment  
Work Package leader: CSMUC  
Lead beneficiary: CSMUC  
Dissemination level: PU  
Nature: Report  
No of pages (incl. cover):

Abstract	The objective of D4.5 is to describe VAMDC Infrastructure Deployment activities during the whole project. This report corresponds to Activities in WP4: SA1 “Infrastructure Deployment”.
----------	--

## Versioning and Contribution history

Version	Date	Reason for modification	Modified by
V0.1	Dec 2012	Preparation of document	M.L. Dubernet
V0.1	Dec 2012-	WP4 report	G. Rixon
	Fev 2013	Final Historical Report	G. Rixon
V1.0	Fev 2013	Inclusion in D4.5	ML Dubernet

Final Version (v1.0) released by		Circulated to	
Name	Date	Recipient	Date
M.L. Dubernet	12 <sup>th</sup> February 2013	Mr Bodo	12 <sup>th</sup> February 2013

**Disclaimer:** The information in this document is subject to change without notice. Company or product names mentioned in this document may be trademarks or registered trademarks of their respective companies.

**All rights reserved:**

The document is proprietary of the VAMDC consortium members. No copying or distributing, in any form or by any means, is allowed without the prior written agreement of the owner of the property rights.

This document reflects only the authors' view. The European Community is not liable for any use that may be made of the information contained herein.

## WP4 ACTIVITIES DESCRIPTION

<b>Work package number</b>	4			<b>Start date or starting event:</b>					3		
<b>Work package title</b>	SA 1: Infrastructure Deployment										
<b>Activity Type</b>	OTHER										
<b>Participant id</b>	1	2	3	4	5	6	7	7	12	13	14
<b>Person-months per beneficiary: (Total = EU + Node Contributions)</b>	66	36	36	12	6	6	8	11	5	9	24

### Table of Content

WP4 activities description .....	5
Table of Content .....	5
1. WP4 Objectives .....	i
2. WP4 Milestones and Deliverables .....	i
3. WP4 Tasks Description.....	i
4. WP4 Tasks Plans for Period 2 .....	<b>Erreur ! Signet non défini.</b>
5. WP4 Tasks Reports for Period 2.....	iv

## 1. WP4 Objectives

To provide Data Access via a homogeneous environment where the distributed user community can retrieve AM resources through a standard interfaces. This involves implementing standard outputs for the AM databases, finding the resources by interrogating registries, using querying and pipeline tools.

WP4 leader is CMSUC (2)

## 2. WP4 Milestones and Deliverables

### Milestones

M4.1	Deployment of Data Access	WP4	CSMUC	Months 10, 22, 34, 42	
M4.2	Deployment of Infrastructure	WP4	CSMUC	Months 10, 22, 34, 42	
M4.3	Evaluation of Available Software	WP4	CSMUC	Months 10, 22, 34, 42	Testing by Users Panels of prototype software
M4.4	Open Call for New Resources	WP4	CSMUC	Months 24	Text of Call Available on Public Website

### Deliverables

***D4.1 Infrastructure Deployment Plan (PM 3)***

***D4.2 Infrastructure Deployment Report to be included in report to the EU – Year 1 (PM 10)***

***D4.3 Infrastructure Deployment Report to be included in report to the EU – Year 2 (PM 22)***

***D4.4 Infrastructure Deployment Report to be included in report to the EU – Year 3 (PM 34)***

***D4.5 Final Report of Service Deployment to be included in final report to the commission (PM41)***

***Annual Infrastructure Deployment Plan revisions included in Revised Annual VAMDC Project Plans – Year 1,2,3***

## 3. WP4 Tasks Description

WP4 Leader	G. Rixon (CMSUC)	
Task Number	Leader	Other Partners
1	G. Rixon (CMSUC)	All partners
2	L. Molina (CNRS)	CMSUC (2), IVIC (14), UU (6) + others TBD
3	K. Benson (UCL)	CNRS (1), UU (6), RFNC-VNIITF (12)
4	ML Dubernet (CNRS)/G. Rixon (CMSUC)	UU(6), UCL (3), KOELN (7)

5	M. Doronin (CNRS)	UU(6), UCL (3), KOELN (7)
6	M.L. Dubernet (CNRS)	All partners

### Description of work

The VAMDC infrastructure will be designed as an homogeneous environment where any AM producer or "community" users will be able respectively to publish their AM data or to retrieve and manipulate those data. The AM producers range from atomic physics to molecular physics handling complex molecules, solids and surfaces. The communities encompass astrophysics users from very different areas: stellar, galaxies, interstellar medium (those application areas are handled by the IVOA and Euro-VO projects), planetology and small bodies of the solar system (EuroPlanet Project), solar-earth system (EGSO and SPASE projects), atmospheric users (studies of earth atmosphere), environmental and combustion chemistry, fusion physics and industrial applications. The IVOA community is the most advanced project as far as building an interoperable infrastructure for astronomy and we will use some of their achievements, i.e. standards, tools, services when those are relevant to the project.

#### **Task 1: Standard access to AM data (lead by CMSUC(2), all SA1 partners)**

We will provide standard service interfaces to AM databases. JRA1 will define these interfaces and this task is to implement them on the existing databases held by each VAMDC node. Participants at all nodes will be involved.

#### **Task 2: Standard access to numerical codes (lead by CNRS(1), with partners (2), (6) )**

Where a VAMDC node has a useful numerical code for AM analysis or modelling, we will make it available as a service. These services will provide a uniform way of launching the codes and recovering their outputs. This task is complementary to the grid adaptation of code in SA2: the codes run on resources contributed by the node owners and need not be made portable to an external grid.

#### **Task 3: Implementing registries (lead by UCL(3) with partners (1), (6), (12))**

The registry facilities defined by JRA1, and implemented with the software produced by JRA2, must be populated with information. This task gathers the meta data for the services at each node and adds it to the registries.

#### **Task 4: Augmenting VODesktop (lead by UCL(3))**

The EuroVO's VODesktop is a generic interface for the virtual observatory. It allows access to all VObs data, plus launching numerical codes and sharing of data between desktop visualization tools. We will adapt A-M desktop applications to work with VODesktop and the underlying VObs applications environment.

**Task 5: Publishing desktop software (lead by CNRS(1), with partner (5))**

We will collect and make available to end users chosen A-M applications for the desktop.

**Task 6: Expansion of the infrastructure (co-lead by CNRS(1) and CMSUC(2) with (5), (6))**

Once the core infrastructure is deployed, new resources will be included in the infrastructure via an open call to producers of AM resources. Those new resources will need to be deployed and tested within the infrastructure. Task 6 will be devoted to the technical inclusion and testing of these new AM resources. The choice of these resources will be made in NA1 by the VPB by the EPT.



## 4. WP4 Final Tasks Reports -

**Period:** 01/07/2009 – 31/12/2012

**WorkPackage:** WP4 – SA1 Infrastructure Deployment

**WorkPackage Leader and co-Leader:** G. Rixon and A. Shih

Participants in the WorkPackage: CNRS, CMSUC, UCL, OU, UNIVIE, UU, KOLN, INAF, RFNC-VNIITF, IAO, IVIC

Part 1

### 1. INTRODUCTION

VAMDC has built an internet infrastructure giving researchers coordinated access multiple to databases of atomic and molecular data. This infrastructure consists in software developed by the VAMDC project and deployed as web applications and web services at member institutions.

This report records the history of deployments and system releases by which the infrastructure was built up over the course of the VAMDC project. At the end of the project, maintenance of the infrastructure is continued by the member institutions supported by the successor project SUP@VAMDC. Therefore, the infrastructure continues to evolve.

### 2. VAMDC ARCHITECTURE

VAMDC infrastructure consists in web services and web applications. In this report, “web service” means a collection of web resources arranged for access from a software application, while “web application” means a collection of dynamic web-pages arranged to form a user interface when accessed by a user's web browser. Some VAMDC installations contain both web services and web applications. All resources in VAMDC web services and web applications are accessible by HTTP.

### 3. Data nodes

VAMDC provides one web service for each database of science data. The combination of the web service and the database is called in the jargon a “VAMDC node”, and the software operating the service, written by VAMDC, is called “node software”.

VAMDC nodes are distributed across the member sites; centralization of the data has been explicitly avoided. Typically, a node is deployed where there are researchers curating the node's database, with a mirror of the service and database at another site to increase the service availability. Nodes and their mirrors can occasionally be moved between sites.

VAMDC nodes provide a query protocol. A clients sends to a node a query to select an extract from that node's database; the node computes the extract and returns it in XSAMS<sup>1</sup> format. The query language is VAMDC SQL subset 2<sup>2</sup> (VSS2) and the query protocol is called VAMDC-TAP.<sup>3</sup>

1 See <http://www.vamdc.org/documents/standards/dataModel/vamdcxsams/index.html>

2 See <http://www.vamdc.org/documents/standards/queryLanguage/index.html>

Because the extracts are computed on demand, all nodes store their data in a relational database rather than in flat files. Constructing the relational form of the database is a major part of deploying a VAMDC node.

All nodes follow the same query protocol, and all present the same, relational data-model established in the VAMDC dictionary. This allows an application to send the same query to all nodes in VAMDC and to aggregate the results. However, the kinds of data available vary from node to node. A node containing only atomic data, for example, will reject a query selecting on molecular quantum-numbers. The protocol allows the client to distinguish these cases from outright failure of a node.

The VAMDC-TAP protocol is designed for direct use by applications. If the VAMDC infrastructure were reduced to just the set of data nodes, then it would be still be usable; the rest of the infrastructure helps but is not essential. This approach was chosen at the start of the project to increase the chance that VAMDC remained useful after the end of funding.

## 4. Registry of services

The VAMDC registry is a database of metadata describing VAMDC nodes and web applications. It allows an application to find the address of a given node; to select nodes by the kinds of data they offer; to find out which query terms are supported at a node. In short, the registry helps applications form correct queries.

A VAMDC system has exactly one registry, set up as a mirrored pair of services (for higher availability) with published, unchanging addresses. If an application knows the address of the registry, it can find all parts of the system even if those parts are migrated between sites.

The VAMDC registry follows the IVOA<sup>4</sup> registry protocol and is built from the AstroGrid<sup>5</sup> registry software. Some aspects of the format of registrations are VAMDC extensions to the IVOA standards.

## 5. XSAMS-processing applications

VAMDC data-nodes produce data extracts in XSAMS format, which is a good data-transfer format but needs to be translated into the native format of applications that consume the data. There is also a need to display data in XSAMS for human assessment.

VAMDC provides a suite of services that transform XSAMS into other forms. These installations are web services conforming to the VAMDC protocol for XSAMS consumers<sup>6</sup>, and some include web applications for interactive use.

The XSAMS-processing services may be discovered in the VAMDC registry.

The commonly-used XSAMS-processing applications were written by VAMDC, but other groups can write and register their own XSAMS processors.

## 6. Web portal

As noted above, the VAMDC nodes can be used directly from application software. For exploratory use, in connecting applications to VAMDC and as an introduction to new users, VAMDC provides one, generic application for querying the nodes and

---

3 See <http://www.vamdc.org/documents/standards/dataAccessProtocol/index.html>

4 See <http://www.ivoa.net/Documents/>

5 See <http://www.astrogrid.org>

6 See <http://www.vamdc.org/documents/standards/dataConsumerProtocol/index.html>

displaying the results. This is a web application, called the VAMDC web portal.

The portal is new software written by VAMDC.

The portal web-application handles the query process but does not handle the data resulting from the query. Instead, the portal allows users to download data directly from the VAMDC nodes, or to pass those data from the nodes to the registered, XSAMS-processing applications. The latter applications provide a way for user-communities to extend the VAMDC portal with special features.

## 7. Database of species

Many queries select by atomic and molecular species, and the names for species vary between scientific communities. VAMDC maintains a database of names from which community-specific terms may be refined into standard identifiers understood by all VAMDC nodes.

VAMDC identifiers are based on InChI codes. In most cases, the VAMDC identifier is just the standard InChI, but in special cases a suffix is added to distinguish molecular conformers.

One copy of the species database is encapsulated in the web portal. Another copy is available for query by applications as a VAMDC data-node. The database is not distributed to software authors outside VAMDC.

## 8. VERSIONING THE VAMDC SYSTEM

VAMDC made (and SUP@VAMDC will continue to make) coordinated<sup>7</sup>, periodic releases of the standards noted in the architecture description above. VAMDC deployments using different versions of the standards are not compatible.<sup>8</sup> Therefore, VAMDC deployments are grouped into separate systems, with one system per release of the standards.

The version of a VAMDC system is the version of the ruling standards, expressed as the year and month (e.g. 12.07 standards were released in July 2012) of the release of those standards. The release date of the system lags the release date of the standards by at least one month.

VAMDC aims to keep two system versions available concurrently: one current release and the release most recently superseded. Software written outside VAMDC for a given release of VAMDC will continue after that release is superseded for at least one more release-cycle, giving the authors of the software more time to update their code to current standards.

A system release contains a set of data nodes (the URLs of the nodes change across releases), a registry, a compatible version of the web portal and a set of XSAMS-consuming services adapted to the correct version of XSAMS. Any software application using a registry from a particular release is guaranteed to see only compatible services from that release; to upgrade to the next release, the software authors must use a different registry.

## 9. PERIOD 1: EARLY PROTOTYPES

At the start of period 1, VAMDC had data but no standards. The first prototypes for VAMDC services were made using IVOA standards.

---

<sup>7</sup> This is in marked contrast to other movements such as IVOA where participating installations upgrade their services piecemeal.

<sup>8</sup> The greatest incompatibility comes from changes in the XML schema defining the XSAMS format.

Several of the existing databases held by VAMDC members (CDMS, Chianti, BASECOL) were set up as Table Access protocol (TAP)<sup>9</sup> services following the IVOA standard and using software inherited from AstroGrid and EuroVO-Tech. These allowed early experiments with little investment in software but were never intended to be part of the final system.

Early in the period, the IVOA standards for the registry were adopted and a registry was deployed at MSSL. Initially, this registry listed the TAP services and the pre-existing web-sites for the members' databases.

The need for a central web-portal was recognized and two prototype portals were deployed. Both were engineering experiments to explore the scope of the problem and were never intended for end users.

A Level-1 “release”<sup>10</sup> of the system was produced from the TAP services, registry and portal prototypes. This gave some visibility of the experiments at the period-1 review but was clearly unsuitable for end users. This release was never publicized outside VAMDC.

Experience with the TAP prototypes showed a need for specialization. XSAMS was specified as the standard output-format in place of IVOA's VOTable. The query language was changed to a different sub-set of ISO SQL, later called VAMDC SQL Sub-set #1 (VSS1). Standard terms for the queries were defined in the VAMDC dictionary. This specialization of IVOA TAP was first termed TAP-XSAMS (renamed VAMDC-TAP in a later period).

Five nodes (VALD, CDMS, BASECOL, UdFA, HITRAN) were deployed using prototype software implementing TAP-XSAMS. A modified version of the prototype portal was deployed to match these nodes.

## 10. PERIOD 2: INCREASING STANDARDIZATION

During period 2, the VAMDC standards were refined. The first, co-ordinated issue of the standards was made as the 11.05 and 11.07<sup>11</sup> releases. The latter release introduced a revised query language, VAMDC SQL Sub-set #2 (VSS2).

The VAMDC-TAP protocol was extended to support a “preview” query to which the nodes reply quickly with metadata. This allows quick, iterative refinement of queries and the web portal was redesigned to emphasize this feature.

More nodes were added to the emerging system: Chianti, GhoSST, KIDA, Toulouse/Cagliari PAH database, LASP, Spectr-W3, CDS, ICB methane database, ICD ethylene database, S&MPO and Lund atomic database. All nodes were considered to be prototypes at this time. The completeness and correctness of implementation varied considerably between the nodes.

A level-2 system release<sup>12</sup> was prepared for review. This included the original prototype nodes from period 1, the new nodes from period 2, a registry and the revised web-portal. The system release was formally based on the 11.05 standards, but some components had already been upgraded to the 12.07 standards. Consequently, the system was not properly interoperable, with nodes needing different query-languages and producing different versions of XSAMS.

At this time, the concept of versioned system-releases was introduced, with the intention that later system-releases would be self-consistent.

---

9 See <http://www.ivoa.net/Documents/TAP/>

10 See <http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/VamdcServiceLevelOne>

11 Developed in period 2 and formally released in the first few days of period 3.

12 See <http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/VamdcServiceLevelTwo> .

Despite its inconsistencies and experimental nature, the 11.05 system gave workable access to a significant number of databases. It was therefore made available to invited beta-testers. This system was not publicly released.

## 11. PERIOD 3: MATURITY AND FIRST PUBLIC RELEASE

Early in period 3, the design of the portal and the ergonomics of the system were reviewed by VAMDC developers. The VAMDC-TAP protocol and interaction between nodes and portal were found to be acceptable and this aspect of the system was deemed stable enough for wider deployment. The UI for queries was redesigned and the controls for selecting by species were respecified. The VAMDC species database was introduced at this time. The facilities for displaying data built into the prototype portal were deemed important, but the data handling in the portal causes serious problems of stability. To address this, the concept of separate, XSAM-processing web services was introduced such that the portal itself did not need to load and parse XSAMS documents.

The 11.12 release of standards was issued, including a significant update to XSAMS 0.3 and the new XSAMS-consumer protocol. The existing nodes were mostly updated to the new standard in situ, thereby abandoning the little-used 11.05/11.07 system.

Since the standards concerning data nodes had stabilized, many more nodes were added to the system. The set of nodes at the end of the period is shown in Table 1. This collection of nodes completed the planned access to data suggested in the VAMDC project plan.

**Table 1: nodes included in the 11.12 system at the end of period 3**

Name	Description
<a href="#">Cologne Database for Molecular Spectroscopy</a>	The Cologne Database for Molecular Spectroscopy (CDMS) contains a catalog of radio frequency and microwave to far-infrared spectral lines of atomic and molecular species that (may) occur in the interstellar or circumstellar medium or in planetary atmospheres. The catalog is continuously updated.
<a href="#">ICB Dijon Methane</a>	Calculated line lists for methane ( $^{12}\text{CH}_4$ , $^{13}\text{CH}_4$ and $^{12}\text{CH}_3\text{D}$ ). The data on methane contain the vibration-rotation energy levels, line positions and line intensities in the range from 0 to 6200 $\text{cm}^{-1}$ .
<a href="#">VALD (atoms)</a>	The Vienna Atomic Line Database (VALD) is a collection of atomic line parameters (wavelengths, transition energies and quantum numbers, oscillator strengths, Lande factors, radiative and collisional broadening). This resource is the VAMDC-TAP representation of the atomic data in VALD3.
<a href="#">Carbon Dioxide Spectroscopic Databank</a>	The current version of CDSD-296 consists of 7 most abundant in the Earth's atmosphere isotopic species of the carbon dioxide molecule: 626, 636, 628, 627, 638, 637, 828, covers 5.9 - 12784.1 $\text{cm}^{-1}$ spectral range and contains 419610 lines.
<a href="#">OACT - LASP Database</a>	"Laboratorio di Astrofisica Sperimentale" (Catania-LASp for short) has been active in Catania starting from the eighties. The eldest of the group, after some training at the Physics department of the Catania University, started the activity at the Catania Astrophysical Observatory. Since then and thanks to several funding agencies



	(Consiglio Nazionale delle Ricerche, Italian CNR; Ministero dell'Istruzione, dell'Universita' e della Ricerca, MIUR; Agenzia Spaziale Italiana, ASI; etc.) and to the help of many colleagues (and directors) of the Observatory the LAsp has grown. Today Catania-LAsp means a group of 6 people with permanent position plus some students and guests, a laboratory building equipped with high vacuum chambers, facilities for the deposition of ice films, ion and Lyman-alpha irradiation experiments, many spectrometers in the range from 190 nm up to 200 micron, and also raman spectrographs.
<a href="#">BASECOL</a>	This database, called BASECOL is devoted to collisional ro-vibrational excitation of molecules by colliders such as atom, ion, molecule or electron. It is supervised by an international working group of molecular physicists and astrophysicists involved in the calculations and use of ro-vibrational cross-sections, in order to ensure the continuity and the quality of the database.
<a href="#">TOPbase</a>	TOPbase lists LS-coupling energy levels, gf-values and photoionization cross sections for astrophysically abundant ions ( $Z=1,14$ ; $Z=16$ ; $Z=18$ ; $Z=20$ ; $Z=26$ ) computed in the Opacity Project.
<a href="#">Theoretical spectral database of polycyclic aromatic hydrocarbons</a>	The Cagliari/Toulouse PAH database is a collection of theoretical spectroscopic data about Polycyclic Aromatic Hydrocarbons and carbon clusters. It provides basic geometric characteristics, energetics, harmonic analyses and electronic photoabsorption data. It is maintained by the Astrochemistry group at INAF-Observatory of Cagliari and the Institut de Recherche en Astrophysique et Plan�tologie in Toulouse.
<a href="#">Chianti</a>	Chianti consists of a critically evaluated set of up-to-date atomic data, together with user-friendly programs written in Interactive Data Language (IDL), to analyse the spectra from astrophysical plasmas. The VAMDC interface presents just the data from the Chianti-v7 release.
<a href="#">TIPbase</a>	TIPbase lists fine-structure levels, A-values, collision strengths and effective collision strengths for astrophysically abundant ions, mainly from the Fe isonuclear sequence computed in the Iron Project.
<a href="#">GSMA Reims S&amp;MPO</a>	Calculated line lists for ozone ( $16O_3$ , $16O18O16O$ and $18O_3$ ). The data on methane contain the vibration-rotation energy levels, line positions and line strengths in the range from 0 to 8000 $cm^{-1}$ .
<a href="#">GSMA Reims Ethylene</a>	Calculated data of ethylene ( $12C_2H_4$ ). The data on ethylene contain the vibration-rotation energy levels, line positions and line intensities in the range from 500 to 7500 $cm^{-1}$
<a href="#">GhoSST</a>	
<a href="#">Lund laboratory spectroscopy database</a>	Experimental data for transitions and lifetimes
<a href="#">Stark-b</a>	Database for "Stark" broadening of isolated lines of atoms and ions in the impact approximation
<a href="#">Spectr-W3</a>	The information accumulated in the SPECTR-W3 ADB contains over 450,000 records and includes factual experimental and theoretical data on ionization potentials, energy levels,

	wavelengths, radiation transition probabilities, oscillator strengths, and (optionally) the parameters of analytical approximations of electron-collisional cross-sections and rates for atoms and ions. Those data were extracted from publications in physical journals, proceedings of the related conferences, special-purpose publications on atomic data, and provided directly by authors. The information is supplied with references to the original sources and comments, elucidating the details of experimental measurements or calculations, where necessary and available. To date, the SPECTR-W3 ADB is the largest factual database in the world containing the information on spectral properties of multicharged ions.
<a href="#">Water internet Accessible Distributed Information System</a>	Database containing information on water spectras, notably data on H <sub>2</sub> 16O, HDO, D <sub>2</sub> O, H <sub>2</sub> 17O and H <sub>2</sub> 18O.
<a href="#">HITRAN-UCL resource</a>	The HITRAN database - truncated version for beta testing, from <a href="http://www.cfa.harvard.edu/HITRAN/">http://www.cfa.harvard.edu/HITRAN/</a>
<a href="#">VALD sub-set in Moscow (obs)</a>	The part of Vienna Atomic Line Database (VALD) with accurate wavelength and energy levels. It also provides laboratory and calculated transition probabilities, Lande factors and broadening parameters. It is used for line identification and spectral synthesis.
<a href="#">KIDA: VAMDC-TAP interface</a>	KIDA is a database of kinetic data interesting for astrochemical (interstellar medium and planetary atmospheres) studies. In addition to the available referenced data, KIDA provides recommendations over a number of important reactions. Chemists and physicists can add their data to the database.

Three XSAMS-consumer services were released with the 11.12 system. These were: basic tabulation of the contents of XSAMS, as a display aid for the web portal; extract of bibliography from XSAMS, as an aid to authors of papers; conversion of XSAMS data to the input format for the application “Spectroscopy made easy”, an application adaptor used in an example of application-workflow published by VAMDC.

In this period, a new version of the web portal was deployed in which the display function of the portal was delegated to the XSAMS-consumers. The query UI was completed to match the new design agreed at the start of the period. This completed the development work on VAMDC's web portal.

In the earlier systems, only one copy of each service was maintained. Downtime on a service could block use of VAMDC, particularly when the registry or portal was out of service. A rule was established that all services should be mirrored on at least two or more sites.

During period 3, mirrors were established and tested for the web portal (primary copy at LPMAA, mirror at IoA Cambridge) and for the registry (primary copy at MSSSL, mirror at OPM). Because the portal and registry have well-known addresses, their mirrors are activated by a manual change in the DNS.

Facilities at OPM were set up to mirror the data nodes, and the portal and registry were adapted to use these mirrors, failing over automatically if the primary installation did not respond.

The 11.12 system was opened to users in a public beta-test during March and April

2012. It was finally released for end users in June 2012 and formed the level-3 system<sup>13</sup> submitted to the period-3 review.

## 12. PERIOD 4: CONSOLIDATION

Most of the infrastructure was already in place by the end of period 3, and period 4 was used for refinement of the system. A new set of standards, the 12.07 release, was issued at the start of the period and the new deployments were put into a new system release.

The VAMDC database of species was established as a VAMDC node that can be queried by applications. Previously, the database was only used inside the web portal.

One other new node was introduced: IDEADB<sup>14</sup>. This was also added to the 11.12 system. Otherwise, the set of nodes at the end of the VAMDC project was as given by table 1, above.

Preparations were made to introduce new nodes during the SUP@VAMDC project. These include the JPL spectroscopic database, the NIST atomic database, experimental data on PAH molecules (complementing the theoretical data already in VAMDC) and several databases from the Radiation Damage in Bio-molecular Systems (RADAM) project.

At the close of the VAMDC project the 12.07 system was still undergoing internal testing.

## 13. STATUS AT END OF PROJECT

The VAMDC infrastructure is functionally complete. All the database listed in the original project-proposal<sup>15</sup> have been established as data nodes. The web portal and registry are functional and there is a small set of XSAMS-processing services.

Four system releases have been prepared during the project. One is in public service; one more is in testing for release during February 2013.

The owners of the databases continue to maintain the data nodes. Continuing maintenance has been arranged for the registry and web portal. The SUP@VAMDC project is in place to coordinate upgrades to the VAMDC system until 2015.<sup>16</sup>

VAMDC is still growing. There are no plans to add new kinds of service, but new data-nodes are in preparation and others are planned. Figure 1 shows the growth of the network during the project. There is no indication in these figures that interest in joining the VAMDC network is waning with the end of the VAMDC project.

---

13 See <http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/VamdcServiceLevelThree>

14 Innsbruck Dissociative Electron Attachment Database. See <http://ideadb.uibk.ac.at>

15 IDEADB replaced eMol.

16 One update to VAMDC standards planned in 2013 and another in 2014. Each involve construction of a new VAMDC system.



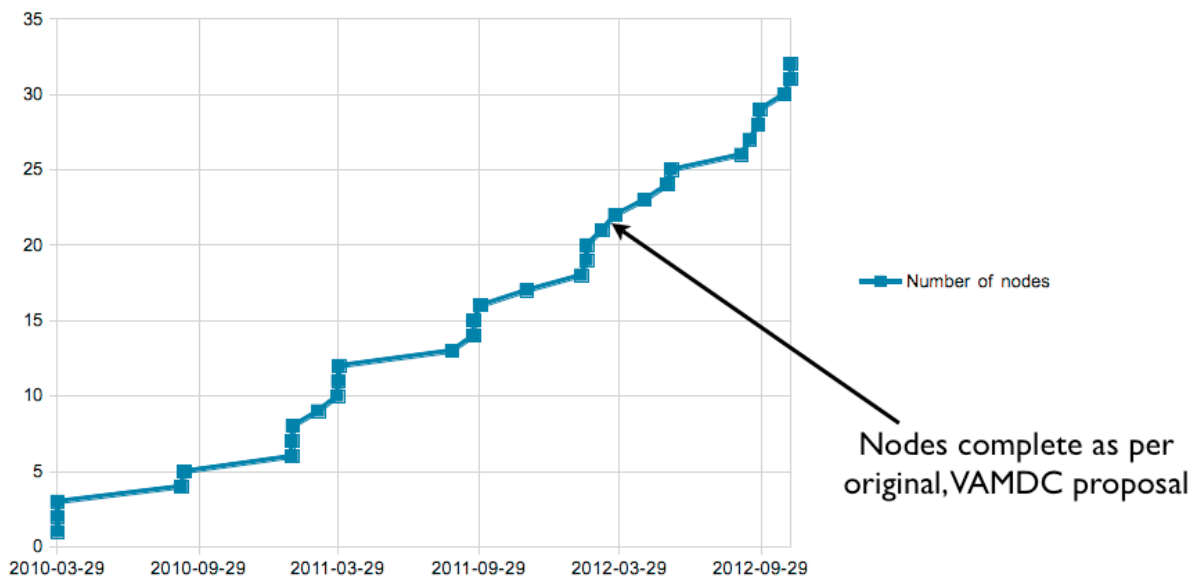


Figure 1: growth of VAMDC infrastructure, by count of data nodes

### Significant results (Activities and Deliverables)

#### Deliverables to EU

**D4.1 Implementation Plan – DONE –**

See <http://www.vamdc-project.vamdc.eu/public-deliverables/16-deliverables-wp4>

**D4.2 Implementation Report to be included in report to the EU – Year 1 – Done –**

See <http://www.vamdc-project.vamdc.eu/public-deliverables/16-deliverables-wp4>

**D4.3 Implementation Report to be included in report to the EU – Year 2 – Done –**

See <http://www.vamdc-project.vamdc.eu/public-deliverables/16-deliverables-wp4>

**D4.4 Implementation Report to be included in report to the EU – Year 2 – Done –**

See <http://www.vamdc-project.vamdc.eu/public-deliverables/16-deliverables-wp4>

**Annual Implementaion Plan revisions included in Revised Annual VAMDC Project Plans – Year 1,2, 3 - See D1.2, D1.5, D1.7** <http://www.vamdc-project.vamdc.eu/public-deliverables/12-deliverables-wp1>

**Internal Deliverables**

- a) System release for 11.12 standards.<sup>17</sup> This system became a final release in July 2012.
- b) Workshop at ICAMDATA, October 2011, for American users and data-providers.
- c) Development and deployment workshop in Paris, July 2012

Deviations from the contract (Annex I) and reasons for them (if applicable)

No Deviations.

Failures to achieve critical objectives and/or not being on schedule and reasons for them (if applicable)

None

Proposed corrective actions (if applicable)

None

---

<sup>17</sup> See <http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/ReleasedNodesAtEndOfPeriod3> for the list of databases at the end of the reporting period. New databases may join this system after the report. This system can be accessed via the web portal at <http://portal.vamdc.eu/>.

