VAMDC

Virtual Atomic and Molecular Data Centre

D1.2

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VAMDC Project Plan

Version 0.5

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:

Beneficiary Number *	Beneficiary name	Beneficiary short name	Country	Date enter project**	Date exit project**
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	ISRAN	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	IVIC	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 supported by funding from the xxxxx Programme under the 7th Research Framework Programme of the European Union

Document

Deliverable number:	D1.2
Deliverable title:	VAMDC Project Plan
Due date of deliverable:	September 2009
Actual submission date:	
Authors:	M.L. Dubernet, N. Walton, N. Mason, G. Rixon, P. Le Sidaner, S. Schlemmer, N. Piskunov, T. Marquart, P. Loboda, A. Fazliev, J. Tennyson, D. Witherick
Work Package no.:	WP1-MGT
Work Package title:	Management Work Package l
Leader:	CNRS
Lead beneficiary:	CNRS
Dissemination level:	PU
Nature:	Document
No of pages (incl. cover):	

Abstract	The objective of D1.2 is to describe VAMDC Project Plan on PM3. It includes the overall project plan as well as the individual packages plans (as described in deliverables D2.1, D3.1, D4.1, D5.1, D6.1, D7.1, D8.1). It provides work details, name of people in charge of board, workpackages, tasks. In addition it gives a short term plan for period 1. It includes the Consortium Agreement as an annexe to the document.

Versioning and Contribution history

Version	Date	Reason for modification	Modified by
V0.1	**19/10/2009**	**First Draft**	**M.L. Dubernet**
V0.2	**20/10/2009**	**Project management**	**M.L. Dubernet**
V0.3	**21/10/2009**	**WP2**	**N. Walton**
V0.4	**21/10/2009**	**WP1, WP2, WP3, WP4, WP5, WP6, WP7, WP8**	**M.L. Dubernet**
V0.5	**01/03/2010**	**WP1, WP2, WP3, WP4, WP5, WP6, WP7, WP8**	**M.L. Dubernet**

Final Version (v0.5) released by		Circulated to	
Name	Date	Recipient	Date
M.L. Dubernet	04/03/2010	Mrs Asero	04/03/2010

EXECUTIVE SUMMARY

The field of atomic and molecular science provides a wealth of data that is used and applied across a wide range of scientific and technological applications. Indeed the progress in many scientific and technological areas is underpinned by the availability of accurate quantitative information on the collisional properties and spectroscopic characteristics of interacting species Atomic and molecular data are indispensable for such diverse applications as astrophysics, atmospheric science, the development of fusion energy, semiconductor manufacturing and other plasma based technologies, the lighting industry, detection and remediation of pollutants (and increasingly the detection of explosives and biological agents as may be used in terrorism) and is essential for understanding many biological processes including modelling radiation damage in cellular systems for therapy treatment. Scientists working with atomic and molecular data are therefore providing foundation for the new era of research – the era of e-sciences. However it is widely recognised that there remain several major challenges to developing a robust and integrated infrastructure that can be used by the widest possible user community. The existing problems can be divided into two categories: (1) data completeness and quality assessment and (2) data interface including problem specific tools for data mining. Today those issues are tackled by a number of data centres but they are highly focussed on specific applications and non-flexible. Thus, there is a strong need to:

1 Develop close links between the user communities, the data producers and data centres based on modern technology.
2 Establish better international coordination in order to promote atomic and molecule data compilation and database activities, avoid duplication of efforts and ensure the use of the best available data.

The Virtual Atomic and Molecular Data Centre (VAMDC) aims at building a secure, documented, flexible, easily accessible and interoperable e-infrastructure for AM data. The VAMDC will be built upon the expertise of existing AM databases, data producers and service providers with the specific aim of creating an infrastructure that on one hand can directly extract data from the existing depositories while one the other hand is sufficiently flexible to be tuned to the needs of a wide variety of users from academic, governmental, industrial communities or from general public both within and outside the ERA. The project will address the building of the core consortium, the deployment of the infrastructure and the development of specific software as well as providing a forum for training of potential users and dissemination across the ERA. It is expected that VAMDC becomes a European legal entity during the course of the project.

Central to this aim is the task of overcoming the current fragmentation of the EU atomic and molecular database community. VAMDC will accomplish it:

- through the development **of the largest and most comprehensive atomic and molecular e-infrastructure** to be shared, fed and expanded by all EU A&M scientists and
- **by providing a major distributed European infrastructure** which can be accessed, referenced and exploited by the wider European Research community.

In fulfilling these aims the VAMDC project will organise a series of **Networking Activities (NAs)** laying the foundations for a long-lasting and self-sustaining Infrastructure. NAs are specifically aimed at

- Engaging data providers
- Coordinating activities amongst existing database providers
- Ascertaining and responding to the needs of different user communities
- Providing training and awareness of the VAMDC across the international community and community of planetary sciences in Europe.

The main output of the VAMDC is the provision of the VAMDC e-science platform delivered through a set of three Service Activities (SAs)

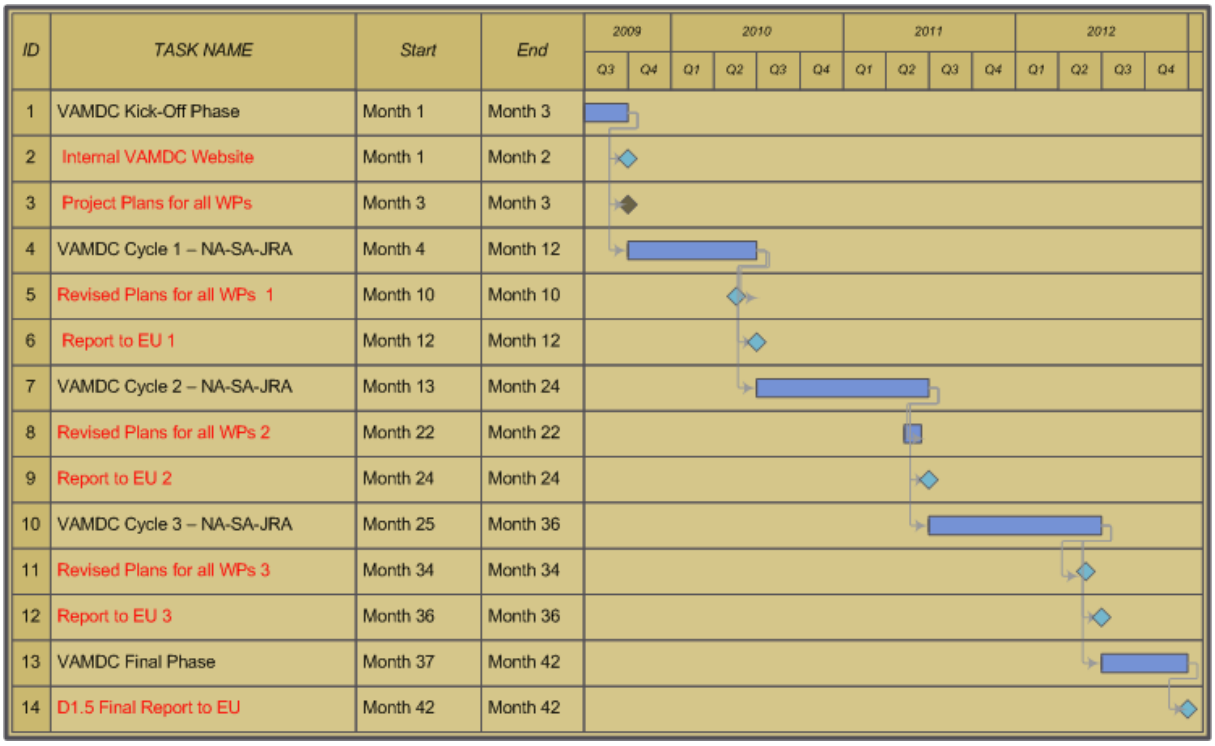
The interoperability and thus the building of an e-science platform on atomic and molecular data require both technical research and development activities as well as scientific involvement of the producers community in order to define specifications, to prepare and to document their data. **VAMDC's Joint Research Activities (JRAs)** will develop this infrastructure improving the breadth and quality of facilities, models, software tools and services offered.

The major aim of VAMDC e-infrastructure is to provide an integrated access to the comprehensive set of A&M databases needed for research across the European Research Area. Management is provided by **WP1.** The core of the project is the creation of two focused services to provide 24/7 access to a large remote service facility e-infrastructure- the **Virtual Atomic and Molecular Data Centre (VAMDC) -** dedicated to the archiving, manipulation and modelling of data collected from past and future A&M research. The two central work packages are therefore WP4 (SA1) VAMDC Service Deployment: WP5 (SA2) VAMDC Infrastructure Support. Although all the databases chosen for inclusion in the E-infrastructure already are operational (see 1.2), several research projects are required to combine them into a single access infrastructure. Thus SAs will 'roll out' over the course of the project as the JRAs improve the services of the integrated infrastructure. The JRAs are: JRA1 (WP6) Ensuring interoperability of the databases; JRA2 (WP7) Developing tools to publish A. & M. Data and JRA3 (WP8) Developing new mining and Integration Tools. It should be stressed that since this is a call for **a Collaborative Project and Coordination and Support Action for ICT based e-Infrastructure** we do not offer a fully functional e-infrastructure at the start of the project but rather will develop the e-infrastructure throughout the project integrating JRAs and SAs whilst being informed both by data provider and user communities (NA1 and NA2). Indeed the whole project will be critically reviewed by a user and expert committees, serving also as an advisory board that will influence the future direction of VAMDC both during the course of the 42 months project and, crucially, beyond as VAMDC becomes a self sustaining infrastructure with a leading role in the ERA. Thus the project is inherently dynamic and responsive but at the end of the programme will have created a unique e-infrastructure that we wish to be the preeminent service to the International A&M community and its disparate user community.

INTRODUCTION

The project time plan has been arranged on the following schedule; A Three month 'kick-off' or set up period during which both the scientific and administrative programme will be further defined, milestones reviewed and approved, crucially relevant staff appointed and briefed

(only WP1, WP2, WP3 are active). At the end of the Kick-off phase, the project detailed work program for Cycle 1, and the Project Web site is available. The main project time plan is then arranged in three cycles, with the project's progress reviewed at the end of each cycle. The first cycle is designated as lasting 9 months, the other two operating over 12 months. A Final Phase of 6 months is planned during which the VAMDC e-infrastructure is envisaged to be a fully active service for 3 months, with a final wrap-up of 3 months where only WP1, WP2, WP3, WP4,WP5 will be active.



ID	TASK NAME	Start	End
1	VAMDC Kick-Off Phase	Month 1	Month 3
2	Internal VAMDC Website	Month 1	Month 2
3	Project Plans for all WPs	Month 3	Month 3
4	VAMDC Cycle 1 – NA-SA-JRA	Month 4	Month 12
5	Revised Plans for all WPs 1	Month 10	Month 10
6	Report to EU 1	Month 12	Month 12
7	VAMDC Cycle 2 – NA-SA-JRA	Month 13	Month 24
8	Revised Plans for all WPs 2	Month 22	Month 22
9	Report to EU 2	Month 24	Month 24
10	VAMDC Cycle 3 – NA-SA-JRA	Month 25	Month 36
11	Revised Plans for all WPs 3	Month 34	Month 34
12	Report to EU 3	Month 36	Month 36
13	VAMDC Final Phase	Month 37	Month 42
14	D1.5 Final Report to EU	Month 42	Month 42

1. PROJECT MANAGEMENT

VAMDC is a complex project involving 15 administrative partners representing 24 teams from 6 European Union member states, Serbia, the Russian Federation and Venezuela. It embraces on the one hand scientists from a wide spectrum of disciplines in atomic and molecular (AM) Physics with a strong coupling to the users of their AM data (astrochemistry, atmospheric physics, plasmas) and on the other hand scientists and engineers from the ICT community used to deal with deploying interoperable e-infrastructure.

The project has several dimensions:

- **Networking Activities** will coordinate the infrastructure activities among all trans-disciplinary fields) both within the ERA and externally through direct partnerships with the Russian Federation, Serbia and Venezuela. The NAs will link VAMDC to other international projects relevant to VAMDC (e.g. Astrogrid, ITER and Europlanet) thus creating a world-wide e-science environment for atomic and molecular data. NA1 will interact with other data providers and ICT teams from both EU and non-EU countries in order to ensure the most comprehensive and inclusive development of the infrastructure. NA2 will disseminate VAMDC services and facilities by engaging and obtaining feedback from anticipated users such as the astrophysics, atmospheric, fusion, ICT communities. The NAs will also have a political role defining the policies

of the infrastructure.

- **Service Activities (SAs)** will create a unique, state of the art e-infrastructure, the **Virtual Atomic and Molecular Data Centre (VAMDC)** for both A&M data producers and users through the availability of major databases in an interoperable format, the maintenance of services allowing publications of small datasets by producer's teams, the maintenance of registries and dictionaries, the maintenance of nodes listing the needs for the various communities (in relation with other EU initiatives) and the creation of a GRID environment for codes and databases.
- **Joint Research Activities (JRAs)** will build the complete set of "tools" necessary to create the VAMDC e-science platform, creating new specifications and creating/adapting/integrating new software.

The success of the project will depend on the effective management and integration of these diverse elements while the programme of work calls for an efficient management structure, designed to deal with the strong interdisciplinary aspect of the project, as well as with all administrative and technical aspects. Management of the technical aspects of the programme is particularly important since the project is focused on delivering the SAs services to support both Partners and external users. This is considered fundamental if VAMDC is to build-up of a community of users capable of taking advantage of the developed know-how and of exploiting it for their own specific goals.

The key values of the management approach we have adopted are:
• **Excellence**. At every level and in every part of the project, we are driven by a commitment to scientific excellence in everything we do. All project activities will be monitored and benchmarked against international standards of scientific excellence under the supervision of the Project Management and Strategic Advisory Boards.
• **Inclusiveness**. To maintain the engagement and commitment of all participants, we believe it is essential that they should feel a sense of shared ownership and responsibility for the project as a whole, not just the part with which they may be directly involved. Agenda and minutes of all project meetings will be available in a private area of the project website. All participants will be encouraged to contribute ideas and opinions on issues under discussion in the Executive and Project Management Board. Users will contribute recommendations to the User and Producer Advisory Committee.
• **Responsiveness**. Resources must be targeted where they will have the greatest impact and used in the most effective way to achieve the project's goals. The proposed structure will therefore ensure close oversight of the individual project elements and the ability to redirect resources as changing circumstances may require. By devolving operational control to the Work Packages we will ensure effective use of resources. At the level of the project as a whole, the Strategic Advisory Board will play an important role in reviewing the achievements and future direction of the project.
• **Transparency**. Decisions must be made, and be seen to be made, against clear and relevant criteria for the benefit of the project as a whole after necessary consultation with those concerned. A professional Project Manager will ensure the availability of up to date and consistent information to inform the decisions of the Project Management Board and the Executive Board.
• **Timeliness**. Decisions must be made in a timely manner or opportunities will be lost. The combination of a devolved structure operating under a strong Executive Team will ensure this.

• **Accountability**. The scientists and others implementing the project must have clear roles, responsibilities and lines of reporting to ensure the effective delivery of the project to time and budget. We have embedded these values at all levels of the project management structure.

2. IMPLEMENTATION PLAN

2.1 Management Structure

The variety of tasks to be carried out within VAMDC, the diverse nature of atomic and molecular processes, the diverse user communities, and the necessary links to other international project requires a good level of coordination as well as harmonisation and control both over the development of research activities and the provision of services. The management scheme has been designed accordingly. The main elements of the structure are:

VAMDC Executive Board (VEB): Comprising the Coordinator of the Network, a Project Manager (to be funded by the e-infrastructure and based at the Coordinator's institute), a scientific co-chair and a technical co-chair. The Executive Board will act as the 'daily' project management team with responsibility for monitoring the progress of the VAMDC e-infrastructure and ensure decisions taken at the Project Management Board are implemented. Such a small team is necessary to deliver clear and decisive management on short time scales. The VEB will also act as the direct point of contact for the Commission. The VEB will be delegated necessary powers by the VPB to act on issues that require immediate response but will be answerable for such actions to the VPB.

VAMDC Project Board (VPB)

This Board will be the major strategic decision-making body and will have the prime responsibility for ensuring the success of the project and compliance with the terms of the EU Contract. Membership will consist of:

- one representative from each legal entity signing the contract (Contractual Legal Entity: CLE) , i.e. the nominated 'Scientist in charge' as defined by the contract,
- representatives of the departments within a CLE when they have quite distinct roles within the proposal,
- representatives of members of a CLE when it is composed of several members, each of which being a separate legal entity (eg CNRS).

The VPB has final control of the budget and the allocation of tasks and resources. The VPB will meet twice a year face-to-face and at other times (as required) by teleconference and will be chaired by the Coordinator. List of VPB members are given in Annexe 6 of Consortium Agreement.

Strategic Advisory Board (SAB).

The SAB will bring together influential international scientists, producers and users of data, as well as representative from international standardisation organisations, with interests

relevant to the project, but who are independent of it. It will ensure that the project is engaged with and responsive to developments in Europe and non-EU countries. It will have an important role in ensuring the project achieves its intended impacts in terms of structuring the European Research in connection with non-EU initiatives and International standards, having the power to co-opt/appoint members from other EU/non EU projects with whom VAMDC wishes to engage. It may also elect selected users of VAMDC e-infrastructure to ensure their feedback on service provision and future service development.

Name	Field	Institute
L. Rothman	Molecular Line Shapes and LineLists, Atmospheric Physics	CFA, Harvard, USA
B. Braams	Atomic Physics, Fusion,	IAEA, Atomic Division, Vienna
6 other Members TBD		

Executive Project Team (EPT)

The Executive Project Team includes the leaders of all WPs: the Dissemination and Training (WP3) activities, the Service Deployment (WP4) and Infrastructure Support (WP5) activities, and all Joint Research Activities (WPs 6, 7, 8). In case of need, each WP leader may be represented at Team meetings by a nominated deputy with voting rights. The EPT will be chaired by the VAMDC Technical Coordinator who is a member of the Project Board and who will appropriately advise the VPB on the technical validity and relevance of the project strategic plans. The Executive Project Team is the core of the management structure from the technical point of view, making sure that the project WPs have a common view and that planned work is well coordinated with other similar international projects. The EPT is planned to be quite operative, thus it will have monthly teleconference meetings (more if necessary) as well as bi-annual face-to-face meetings. The EPT will collect reports from SAs and JRAs and prepare the annual technical reports for the VPB. The Project Coordinator will have a standing invitation to participate in the meetings.

Role	Name	Partners
Chair	N. Walton	CMSUC (2)
Co-Chair	J. Bureau	CNRS: LPMAA (1)
WP3 Leader/ deputy Leader	N. Mason / F. Kupka	OU(4), UNIVIE(5)
WP4 Leader/ deputy Leader	G. Rixon / A. Shih	CMSUC(2), CNRS: UMS (1)
WP5 Leader/ deputy Leader	P. Le Sidaner / K. Benson	CNRS: UMS (1), UCL: MSSL (3)
WP6 Leader/ deputy Leader	S. Schlemmer / M.L. Dubernet	KOLN (7), CNRS: LPMAA/LUTH (1)
WP7 Leader/ deputy Leader	N. Piskunov / U. Heiter	UU (6)
WP8 Leader/ deputy Leader	J. Tennyson / D. Witherick	UCL: PA (3)

Communication and Training Committee (CTC)

The CTC will organise a series of dissemination and training actions in WP3. The CTC will be composed of the Partners involved in WP3 and chaired by the WP3 leader. Its Chair is a member of the EPT, she/he has the right to attend the VPB and to speak to issues raised by the CTC.

Role	Name	Partners
Chair	N. Mason	OU (4)
Co-Chair	F. Kupka	UNIVIE (5)
Members	8 members TBD	CNRS (1), CMSUC (2), UCL (3), UU (6), KOLN (7), AOB (10), IAO (13), CPTM (14)

2.2 Management Roles

Agreed at kick-off Meeting: Role

Role	Name	Partners
Project Coordinator	M.L. Dubernet	CNRS : LPMAA/LUTH (1)
Scientific Deputy Coordinator	N. Mason	OU (3)
Technical Deputy Coordinator	N. Walton	CMSUC (2)
Project Manager	J. Bureau	CNRS (1)

Agreed at kick-off Meeting: Work package Leaders

WP Number	WP Leader	WP deputy leader	Partners
WP1: MGT	M.L. Dubernet		CNRS:LPMAA/LUTH (1)
WP2: NA1	N. Walton	J. Bureau	CMSUC (2) / CNRS:LPMAA (1)
WP3: NA2	N. Mason	F. Kupka	OU (4) / UNIVIE (5)
WP4: SA1	G. Rixon	A. Shih	CMSUC (2)/ CNRS: UMS(1)
WP5: SA2	P. Le Sidaner	K. Benson	CNRS:UMS (1) / CMSUC (2)
WP6: JRA1	S. Schlemmer	M.L. Dubernet	KOLN / CNRS:LPMAA/LUTH (1)
WP7: JRA2	N. Piskunov	U. Heiter	UU (6) / UU(6)
WP8: JRA3	J. Tennyson	D. Witherick	UCL (3) / UCL (3)

The key roles within the VAMDC management structure are:

The VAMDC Project Coordinator. The Project Coordinator will have overall executive responsibility for the project and will provide leadership. Professor Marie-Lise Dubernet (CNRS) will fill this position. The Coordinator chairs the Project Board and she will have a standing invitation to participate in the meetings at the EPT. The Coordinator will have prime

responsibility for representing the project externally, including liaison with the European Commission..

The Scientific Deputy Coordinator. The Scientific Deputy Coordinator reports to the Coordinator and has prime responsibility for ensuring the scientific coherence of the project and the quality of its outputs. (S)he will work closely with the Work Packages leaders on scientific matters and on planning the future direction of the project. The Scientific Deputy Coordinator will also work closely with the Strategic Advisory Board to assure quality of delivery. The Scientific Deputy Coordinator will be a leading scientist appointed by the VAMDC Project Board on the recommendation of the Coordinator from the partners and will have to be able to commit a substantial fraction of his/her time per week to VAMDC business.

The Technical Deputy Coordinator. (S)he is in charge of the overall coordination of the various technical activities and he is the Chair of the Executive Project Team (EPT). For maximum efficiency in communication s(he) will be the co-chair of the S/T Coordination Work Package (WP2: NA1).

Project Manager. The Project Manager has detailed oversight of all Work packages. (S)he will ensure regular monitoring of progress against milestones and budgets, giving early warning of areas where problems may occur. The Project Manager will be the project's Chief Operating Officer, preparing agenda for the VAMDC Project Board and EPT and implementing their decisions, including the distribution of the EU Grant and the compilation of reports and other data required by the European Commission. The Project Manager will be appointed by the Coordinator and will be employed by the Coordinator's organisation.

Work packages Leaders. Work packages leaders will have day-to-day responsibility for achieving the milestones and deliverables of their Work packages within agreed time scales and budgets. They will monitor and report progress through the Project Manager and identify issues that may impact the project as a whole. With the Scientific Director, WP Leaders will assure the quality of deliverables. To mitigate risk and share work loads each WP also has a deputy appointed.

Chair of the Communication and Training Committee. The chair of the Communication and Training Committee (Professor N J Mason (OU)) is the Leader of the Dissemination and Training (WP3) Work package. He has the usual duties of a work package leader (see above) with coordination, timely deliverables and reports to the Project Board. He will also be responsible for proposing yearly dissemination and training actions for approval to the VAMDC Project Board. Once approved these actions will be implemented the following year.

To minimise costs, meetings will be held via teleconference whenever appropriate, although at least three meetings of each group are planned to be face-to-face.

2.3 Description of Beneficiaries (Institute and Key People)

2.3.1 CNRS (Paris, Reims, Grenoble, Bordeaux, Dijon, Toulouse)

The Centre National de la Recherche Scientifique (CNRS) is the largest public multidisciplinary research organisation in France. For this particular project CNRS will concern researchers/engineers from 7 UMR and 1 UMS geographically distributed in 7 institutes: University of Paris 6, Paris Observatory, Bordeaux Observatory (University of Bordeaux I), Grenoble Observatory (University Joseph Fourier), University Champagne-Ardenne, University of Bourgogne and University Paul Sabatier.

French Participants under CNRS (Partner 1)	
Name of the Legal Entity	**Contact Person**
LPMAA, Université de Paris 6, UMR7092	**M.L. Dubernet**
LUTH, Observatoire de Paris, UMR8102	**E. Roueff**
LERMA, Observatoire de Paris, UMR8112	**C. Zeippen & S. Sahal-Bréchot**
VOPARIS Data Centre, Obs. Paris, UMS 2201	**P. Le Sidaner (& M.L. Dubernet)**
LAB, Université de Bordeaux, UMR5804	**V. Wakelam**
LPG, Université Joseph Fourier, UMR5109	**B. Schmitt**
ICB, Université de Bourgogne, UMR5209	**V. Boudon**
GSMA, Université Champagne-Ardenne, UMR6089	**V. Tyuterev**
CESR, Université Paul Sabatier, UMR5187	**C. Joblin**

2.3.1.1 CNRS/LPMAA [Université Pierre et Marie Curie]

LPMAA/UMR7092 is the coordinating JRU of VAMDC project.
LPMAA is a leading laboratory for in situ studies of the Earth Atmosphere, they launch their own balloons in Siberia and Brazil, perform analysis of their spectra and collaborate closely with researchers modelling the earth atmospheres. Some other teams are involved in theoretical spectroscopic activities and have close collaborations with GSMA(CNRS) and IAO (Russian Federation). They are also involved in experiments related to the spectroscopy of CH4 for application to Titan, O3, to the ro-vibrational relaxation of molecules for planetary sciences, to the photodissociation of H2. With the coordinator of the present proposal, LPMAA is now involved in theoretical calculations of ro-vibrational de-excitation rate coefficients for application to interstellar, circumstellar and cometary atmospheres, of line broadening coefficients for application to planetary and earth atmospheres, development of database with BASECOL, Virtual Observatory activities of software design and standards definition. The LPMAA is a laboratory associated to the CNRS and University of Paris 6.

M.L. Dubernet (UMR 7092) Astronomer. She belongs both to LPMAA where she is the UMR director and to Paris Observatory (VOPARIS Data Centre, LUTH).
Expertise: Scientific leader of Virtual Observatory activities at Paris Observatory (scientific PI of VOPARIS Data Centre), activities ranging from VO output of databases, numerical simulations and software development. She has built the VOPARIS Data Centre at Paris Observatory together with Pierre Le Sidaner and has initiated the participation of the Observatory of Paris in EGEE. From training, she is a theoretical molecular physicist specialist of molecular collisional processes. She designed the BASECOL database on inelastic collisions of molecules and is still the scientific PI of the BASECOL database and related web/http services. She is a Member of the Scientific Councils of the French Virtual Observatory and of the National Program "Physics and Chemistry of the Interstellar Medium", as well is the Deputy Coordinator of the FP6-RTN network "Molecular Universe"

(01/10/2004 to 30/09/2008). She has initiated the project of standardisation of the exchanges of atomic and molecular data, works in collaboration with IVOA to produce a Line Data Model, and in collaboration with NIST (Y. Ralchenko), ORNL (US), IAEA (Vienna) to create a XML schema describing atomic and molecular interactions. Her work is at the interface of physics, chemistry, astrophysics, atmospheric physics, software specification and software design.
Role in VAMDC project: M.L. Dubernet is the coordinator of the project (from LPMAA). In addition she will participate to the definition of specifications in JRAs, will advice on deployment of molecular spectroscopy databases (SA1).
J. Bureau (UMR 7092) Research Engineer
Expertise: Scientific Computing, Spectroscopy, Application to Atmospheric Physics
Role in VAMDC project: GRID in SA1 and SA2. Standards in JRA1
M. Delplanque (UMR 7092) Research Engineer
Expertise: Edition of Documents
Role in VAMDC project: Management in WP1 (documents)
F. François (UMR 7092) Assistant Technician
Role in VAMDC project: Management in WP1 (logistics, documents)
S. Tacine (UMR 7092) Assistant Engineer
Expertise: Financial Management
Role in VAMDC project: Management in WP1 (budget)

2.3.1.2 CNRS/ VOPARIS Data Centre, CNRS/LUTH and CNRS/LERMA [Observatoire de Paris]
VOPARIS Data Centre is a federative infrastructure linked to the departments and the computer centre of Paris Observatory. It is strongly involved in Virtual Observatory activities covering many disciplines in astrophysics, molecular physics, solar physics, etc.. VOPARIS Data Centre has a staff of 4 engineer with an infrastructure including computing power linked to the EGEE grid, storage facilities and servers (more information on VOPARIS Data Centre is provided in Section on Resources to be committed).
P. Le Sidaner (UMS2201) Research Engineer, Computer Centre,VOPARIS Data Centre
Expertise: Project Manager of VOPARIS Data Centre and for Vorg at Observatory of Paris
Role in VAMDC project: Infrastructure at VOPARIS Data Centre (network, storage, computing facilities) in SA1 and SA2
A. Shih (UMS 2201) Research Engineer, Computer Centre, VOPARIS Data Centre
Expertise: System Engineer
Role in VAMDC project: Infrastructure at VOPARIS Data Centre (network, storage, computing facilities, Contact with EGEE) (SA2)
A Marchand (UMS 2201) Research Engineer, Computer Centre, VOPARIS Data Centre
Expertise: System Engineer
Role in VAMDC project: User Support at VOPARIS Data Centre (Porting Codes to the GRID) (SA2)
J. Marchand (UMS 2201) Research Engineer, Computer Centre, VOPARIS Data Centre
Expertise: System Engineer
Role in VAMDC project: Infrastructure at VOPARIS Data Centre (network, storage, computing facilities) (SA2)

The **LUTH** (Laboratoire Univers et Théories) is a mixt research unit (UMR 8102) of CNRS, Observatoire de Paris, and Université Paris Diderot. LUTH emphasizes on intensive numerical simulations and interdisciplinarity, two determining aspects of modern research activity in astrophysics. LUTH is strongly implied in the development of the virtual observatory in different domains : VO-Theory, Molecular Physics, High Energy Astrophysics and Exoplanets. These virtual observatory are one of the strategic priorities of Paris Observatory. Services developed at LUTH cover : simulations of the physics of the interstellar medium, large scales simulations in cosmology, molecular data for the spectroscopy in the UV, high energy spectra, exoplanet encyclopedia. Members of LUTH participating to these VO services are often implied both in the development of the services and in the development of the VO standards at international level. LUTH has been involved in Virtual Observatory activities linked to atomic and molecular data.

F. Le Petit - Senior Paris Observatory researcher
Expertise : VO-Theory and Grid computing
Role in VAMDC project: Numerical Codes and Grid Computing (WP4, WP5)
F. Roy - Senior Engineer
Expertise : VO-Theory and Grid computing
Role in VAMDC project: Numerical Codes and Grid Computing (WP4, WP5)
E. Roueff - Senior Paris Observatory researcher
Expertise : Atomic and Molecular standards
Role in VAMDC project: Standards definition (WP6), Publication and Standards Policies (WP2), expert on molecular Physics

The LERMA, department of Paris Observatory, associated to the CNRS, University Paris 6, the Ecole Normale Supérieure and University of Cergy-Pontoise, is an interdisciplinary laboratory covering astrophysical observations and modeling of star forming regions and galaxies, theoretical and experimental atomic and molecular physics as well as instrumentation for Herschel and Alma. Through the activities of the coordinator (M.L. Dubernet) in collaboration with a LERMA software engineer LERMA has been involved in Virtual Observatory activities linked to atomic and molecular data. Members of the LERMA are also involved in atomic databases, as well as in opacity studies in the framework of ambitious national (in collaboration with the CEA) and international (in collaboration with several American and European countries) projects.

C. Zeippen (UMR 8112) Senior CNRS Researcher
Expertise: Calculation of atomic data, atomic data bases, opacity server, astrophysical applications for the interstellar medium and stellar physics. Founding member of the international projects OPACITY and IRON. Management experience: head of the DAMAp department of the Observatory of Paris (8 years), Vice President of the Administrative Council of the Observatoire de Paris (since February 2003).
Role in VAMDC project: expert on atomic data (JRA1), TIPTOPBase (SA1)
S. Sahal-Bréchot (UMR 8112) Senior CNRS Researcher
Expertise: Calculation of atomic data
Role in VAMDC project: expert on line shapes (JRA1), Stark-B (SA1)

2.3.1.3 CNRS/LAB [Université de Bordeaux]

Laboratoire d'Astrophysique de Bordeaux (LAB, UMR 5804) is part of the Observatoire Aquitain des Sciences de l'Univers (OASU, UMS 2567), which groups several laboratories involved in astronomical and Earth sciences. LAB is part of several international astrophysical projects such as ALMA and is currently developing a strong expertise in astrochemistry.
Key persons
V. Wakelam (UMR 5804) Associate researcher, project leader of the KInetic Database for Astrochemistry, scientific leader of the astrochemical dictionary, modelisation of chemical species in interstellar medium, identification of key reactions in chemical networks
A. Caillo (UMS 2567) Research Engineer, development leader of the KInetic Database for Astrochemistry
B. Pavone (UMS 2567) Research Engineer, development of the KInetic Database for Astrochemistry

2.3.1.4 CNRS/LPG [Université Joseph Fourier]

LPG started in 2006 to develop the STSP service that will comprise a set of spectroscopic and physical data bases on several types of solids (atomic and molecular, complex organics, minerals). The current development is focused on the spectroscopic database (spectra and band list) of molecular solids, its associated administration and query interfaces and some related spectroscopic tools. A prototype for band list data will be delivered end of 2008. A preliminary data model covering this field has been developed and will constitute a starting point for the development of a more general data model of physical data on atomic and molecular solids.
LPG will be involved in several WP of this project :
- build the molecular solids physical properties databases (JRA1)

- collection of the users requirements for solid AM data
- develop a molecular physics data model and XML schema for solids, compatible with the current AM data model for gas (JRA1, task 1).
- build dictionaries and registries for solids (JRA1, tasks 2 and 4)
- contribution to the design a general query language for atomic and molecular data (JRA1, tasks 3)
- contribute to adapt the publishing tools to solid AM databases (JRA2), (mostly by expertise on solid DM).
- Contribute to build the query protocols to access published solid AM data (JRA3)
- Develop and install data-access service software at the STSP level. Documentation (SA 1)
- contribute to Quality Assurance of data and resources (SA3, task 2)

Key persons

Bernard Schmitt, DR2 CNRS:

Role in VAMDC project: scientific manager for solid AM databases, user requirements, data models, registries and dictionaries, Quality Assurance and Documentation of data

Pierre Volcke, IE CNRS:

Role in VAMDC project: technical manager, data models, XML Schema, software development, query language and protocols

Non-permanent Staff from CNRS

Role in VAMDC project: Data validation + database feeding

2.3.1.5 CNRS/ICB [Université de Bourgogne]

The Molecular Spectroscopy and Applications group of the Institut Carnot de Bourgogne is the world leader in the analysis of high-resolution spectra of methane ($^{12}CH_4$, $^{13}CH_4$ and CH_3D). It will produce a data base of line parameters for these three isotopologues (positions, intensities, lineshape parameters). Methane is a major greenhouse pollutant on Earth and an important constituent of many astrophysical bodies (giant planets, Titan, dwarf planets, brown dwarfs, methane stars, exoplanets). Modelling methane absorption over a wide spectral range is essential to retrieve methane vertical profiles, minor species abundances and surface properties. It is thus of primary importance for the study of these objects to constitute a highly reliable and consistent database of line parameters extending for the far infrared to the visible region.

Key Persons

V. Boudon (UMR 5209) CNRS Researcher, head of the Molecular Spectroscopy and Applications (SMA) group in Dijon, chairman (2007, 2011, …) and member of the scientific committee of the Colloquium of High Resolution Molecular Spectroscopy

Expertise: Activities concern the modelling of the absorption spectrum of small molecules, especially CH_4, and the production of programs and linelists.

Role in the project: Leader of ICB(CNRS), Member of Project Board, PI of methane line list database (SA1), evaluation (SA2)

T. Gabard (UMR 5209) Associate Professor

Expertise: working on theory and programs for the study of lineshapes of the methane molecule.

Role in the project: producer expert (NA2), evaluation (SA2)

R. Surleau (UMR 5209) CNRS Research Engineer

Expertise: Database management and software design

Role in the project: working on spectroscopy software development (JRA3) and access to methane line list database (SA1)

2.3.1.6 CNRS/GSMA [Université Champagne-Ardenne]

Profile. The Group of Molecular and Atmospheric Spectroscopy (Groupe de Spectroscopie Moleculaire et Atmospherique , GSMA, UMR CNRS 6089) of the University of Reims, France, is the world recognized leader in the analysis and theoretical modeling of high-resolution spectra of ozone. The group has the unique experimental equipment for recording long-path Fourier transform spectra (FTS) in the infra-red and visible range, which over years has been used for producing very accurate data on line positions, intensities and line shape parameters for isotopologues of water, ozone, H2S,

SO2, methane, CO2, acetylene and other molecules. These parameters are used as reference data in various databanks for atmospheric and astrophysical applications.

Information systems.

In collaboration with LTS of Tomsk IOA Institute, GSMA has developed the S&MPO user friendly information system specific for ozone data: "Spectroscopy & molecular properties of Ozone (http://ozone.iao.ru, http://ozone.univ-reims.fr) containing original Reims data in the infrared range. S&MPO is regularly updated including full reference lists classified according fields and allows a direct access and data retrieval. Contrary to traditional databases this information system contains information on molecular properties as well as programs and extended facilities for user applications involving calculations and experimental data. It also contains much more data on ozone then other sources. It includes original experimental cross section ozone data recorded in GSMA in the UV range, which have been recognized as the most accurate ones by the spectroscopic community.

GSMA also participated in SPECTRA atmospheric spectroscopy information system (GIP calculation code), developed in LTS Tomsk, Russia.

Contribution to databases for atmospheric and astrophysical applications:

GSMA is responsible (A.B.) for ozone input parameters to HITRAN /GEISA databases.

In collaboration with ULB the GSMA creates and maintains the most extended experimental "Reims-Brussels database" on high-resolution water lines in the range 4000-25000 cm^{-1}. GSMA provides accurate experimental data on the IUPAC project "A database of water transitions from experiment and theory " (PI: J.Tennyson).

Sofware development :

GSMA develops and explores with collaborators three types of programs: "MULTIFIT" type code for simultaneous experimental spectra processing and accurate measurements of line parameters. GIP type codes for spectroscopic data reduction and modelling. S&MPO type information systems for simulation of absorption/emission.

Role in the project: (A) in the frame of the VAMDC the GSMA together with collaborators will host, maintain and regularly upgrade original data bases and information systems described above including: the ozone data, original experimental long-path experimental line parameters, and newly created database on hydrogen sulphide spectral parameters. (B) GSMA will contribute to the development of tools for the common access to these data, to the expertise and standardisation on molecular and **atmospheric data,** documentation and bibliography.

(C) GSMA will develop the software for the common use of the VAMDC network

in collaboration with IOA Tomsk, Russia aiming at: simulation of absorption / emission high and low resolution molecular spectra for atmospheric applications , visualisation and graphical representation of molecular data for the VAMDC network, intercomparison of various sources of molecular spectroscopy data.

Key Persons

Vladimir Tyuterev, Professor, responsible for the "CH4@Titan" project and "S&MPO" information system from the Reims side, member of the Journal of Molecular Spectroscopy Editorial Board and of the scientific Committee of the HighRus Colloquium.

Expertise: Calculation and modelling of high-resolution spectra of atmospheric species; databases, information systems, molecular dynamics.

Role in VAMDC project: Contact person for GSMA, member of SAB, molecular expert, standards (JRA1), coordination of collaboration with Tomsk

Alain Barbe, Professor, member of the Committee of the OHIO HRMS Colloquium and ASA / HITRAN workshops.

Expertise: Ozone spectroscopy, atmospheric applications

Role in VAMDC project: expert on atmospheric applications, evaluation (SA2)

Michael Rey, CNRS researcher, member of the SPECMO network Committee

Expertise: methane spectroscopy, global spectra calculations

Role in VAMDC project: programming & line list production (SA1), server for S&MPO database

Ludovic Daumont , Associate Professor (MC),

Expertise: experimental long-path spectroscopy of $H_2O/HDO/D_2O$

Role in VAMDC project: Reims-Brussel and IUPAC line lists (SA1), documentation (JRA1), evaluation (SA2)

Laurence Regalia-Jarlot , Accociate Professor (MC),
Expertise: experimental line parameters
Role in VAMDC project: software for simulation of absorption molecular spectra for atmospheric applications and comparison with observed spectra (JRA3)
Marie-René De Backer-Barilly, Professor ,
Expertise: molecular spectra assignment
Role in VAMDC project: upgrading S&MPO ozone line list (SA1), references and documentation (JRA1)
Lilian Joly, Accociate Professor (MC),
Expertise: laser applications, experimental equipment for space missions
Role in VAMDC project: documentation, evaluation of data for laser applications (SA2)
Xavier Thomas, CNRS Research Engineer,
Expertise: FTS instrumentation, spectra recording
Role in VAMDC project: software for simulation of atmospheric molecular absorption (JRA3)
Nicolas Dumelie, Engineer at University of Reims
Expertise: network, programming
Role in VAMDC project: Infrastructure for GSMA servers (network, storage, computing facilities) (SA1)
Maud Rotger, Professor
Expertise: software for databases, molecular data for ethylene
Role in VAMDC project: Graphical tools for the analysis and simulation of high-resolution molecular spectra (JRA3)

2.3.1.7 CNRS/CESR [Université Paul Sabatier]

The Toulouse team is strongly involved in the study of the physics and chemistry of interstellar matter: gas, dust and thier interaction. The team provides an instrumental contribution to ESA space projects (HIFI on board Herschel). The team has also developed an original experimental set-up, PIRENEA for the study of the photophysics and chemistry of large molecules such as Polycyclic Hydrocarbons (PAHs) in physical conditions approaching those of interstellar space. Dr C. Joblin has a wide experience in the study of interstellar PAHs using a multidisciplinary approach that combines observations and laboratory expriments.
Key Persons
C. Joblin (UMR 5187) Senior CNRS Researcher
Expertise: interdisciplinary studies on polycyclic aromatic hydrocarbons (PAHs) and application to astrochemistry, president of the french National Program “Physics and Chemistry of the Interstellar Medium”, task manager in the FP6-RTN network “Molecular Universe”.
Role in VAMDC project: definition of standards for PAH(JRA1), NA1 (tasks: user requirements for PAH), Preservation and Quality Assurance (SA2)
A. Simon (UMR 5187) Research Associate,
Expertise: physico-chemist, experimental and theoretical studies on PAHs and their complexes with heavy atoms (Fe, Si in particular)
Role in VAMDC project: definition of standards for PAH(JRA1), NA1 (tasks: user requirements for PAH), Preservation and Quality Assurance (SA2)
A. Walters (UMR 5187) Professor
Expertise: Spectroscopy in radio-mm-submm-THz
Role in VAMDC project: Evaluation of spectroscopic data (SA2) and definition of standards (JRA1)

2.3.2 The Chancellor, Masters and Scholars of the University of Cambridge (CMSUC)

2.3.2.1 The Institute of Astronomy, University of Cambridge

Profile: The Institute of Astronomy, University of Cambridge enters the project on behalf of the AstroGrid Project, a consortium of seven UK Universities and Public Laboratories Virtual (Universities of Edinburgh, Leicester, Manchester, University College London, Bristol and the STFC's Rutherford Appleton Laboratory). AstroGrid developed the technical infrastructure necessary for the VO, (e.g. Virtual Storage, Authentication, APIs, Workflow systems, and grid and web service interfaces) as well as development of the related standards. AstroGrid is the technology lead partner within the European VO, leads the Euro-VO Technology Centre, and is the coordinating partner for the EC FP6 VOTECH project. AstroGrid, along with CDS, ESO, and the US-NVO, was a founding member of the International Virtual Observatory Alliance (IVOA) and is a member of the EC FP6 Euro-VO Data Centre Alliance and the EC FP7 Euro-VO AIDA projects. From 2009 AstroGrid will be superceded by the VOTC:UK initiative charged with ensuring the continued maintenance and development of its VO infrastructure supporting the community of users, missions and facilities using this software.

The University of Cambridge includes a world class Astronomy research cluster including the Institute of Astronomy (IoA). The IoA conducts front rank research in cosmology, active galaxies, Galactic Structure, and star and planet formation, and is a major user of A+M data. It operates the Cambridge Astronomy Survey Unit (CASU) which develops major science pipelines which are used to generate the science data products for major missions such as the European Southern Observatory's VISTA infrared survey telescope (data rates of >100TB/year). The IoA leads the Photometric processing in the Gaia Data Processing Consortium, and is responsible for one of the main Data Processing Centres for Gaia, ESA's cornerstone astronomy mission (launch 2011). It is a member of the Planck Data Processing Consortium. Cambridge is world renowned for both theoretical and applied computer science, the Computer Lab and the Cambridge eScience Centre being two centres of activity. It hosts the High Performance Compute Facility – the current Darwin machine being the most powerful civilian supercomputer in the UK. AstroGrid and CASU both collaborate actively with this local pool of expertise in Grid and e-Science activities. The IoA has relevant collaborative research links with a number of industrial partners including Oracle.

Role in the project: the IoA, Cambridge will lead SA1, where its technical experience in developing the technical grid and VO infrastructures will be vital in deploying new A+M resources into this infrastructure for the benefit of the A+M communities. In SA1 the IoA will have a key role in defining the standard access systems, resource registration and infrastructure extension. The IoA will also participate in SA2 supporting the continuing service availability, with a ky role in quality assurance of the software and services. Its participation in NA1: Strategy and NA2: Training will focus on providing expertise in technical leadership of VAMDC and leadership in providing technical training to the community in the use of the new research infrastructure.

Key Personnel at the IoA, Cambridge include the principle technical contact, Guy Rixon. is the system architect of AstroGrid. He was until recently (May 2008) Chair of the International Virtual Observatory Alliance working group on Grid and Web Services. In this role he had led and developed the VO systems in interfacing to the Grid and Web services realm. He has played a major role in the development of the authentication and authorisation framework for

the VO, and the VOSpace storage system. Rixon is an acknowledged leader in grid and web service technologies.

The IoA group includes a number of scientists and developers who will contribute to VAMDC with relevant experience in Virtual Observatory and Grid infrastructure. For instance the IoA hosts the Euro-VO Technology Centre Project Scientist and secretary of the IVOA and co-Chair of the Open Grid Forum's astronomical applications Research

2.3.2.1 Department of Applied Mathematics & Theoretical Physics, University of Cambridge

The Cambridge (DAMTP) node consists of Helen Mason (HEM) and Giulio Del Zanna (GDZ). GDZ and HEM are members of the international CHIANTI team. CHIANTI, first released in 1997, is a well-established atomic database (with over 1000 citations) for ions of astrophysical importance. Combined with IDL spectroscopic diagnostic programs, it is used in the analysis of optically thin collisionally-ionised plasmas (it is the reference database in solar physics). The CHIANTI package contains atomic structure data (experimental and calculated wavelengths and radiative data), and rates for electron and proton collisions. The data are obtained from published literature, sometimes supplemented by our own calculations. They are regularly assessed and updated every year or so. References to the original sources are supplied and each version is described in a journal paper. The latest version (6) of CHIANTI, soon to be released (2008), will contain new rates for ionization and recombination, which allows the treatment of non-equilibrium plasmas. The CHIANTI data and programs are distributed via SolarSoft to the solar community, but are also available on the web (www.damtp.cam.ac.uk/user/astro/chianti/) as a large number of ascii files.
CHIANTI atomic data are now also included in many other databases and spectral codes used to study astrophysical plasmas. To make them more accessible, some of the basic atomic data and calculated ones (line emissivities) were imported (VOTADA) into a MySQL database accessible from the Astrogrid Workbench.
The VAMDC project which will enable CHIANTI to be more widely used by the astrophysics and plasma physics communities.

Key Persons

H. Mason (DAMTP, CMSUC), Professor
Expertise: atomic physics, database management
Role in VAMDC project: deployment of CHIANTI (SA1), dissemination (NA2)

Giulio Del Zanna (DAMTP, CMSUC), STFC advanced fellow at UCL
Expertise: atomic physics, database management, tools for astrophysics
Role in VAMDC: deployment of CHIANTI (SA1), dissemination (NA2)

2.3.3 University College London (UCL)

UCL will participate via the Department of Physics and Astronomy (PA) and Mullard Space Science Laboratory (MSSL).

2.3.3.1 UCL/PA

has a staff of about 200 and a turnover in excess of £11M; it has one of the UK's largest atomic and molecular physics group who have a major activity in the provision and curacy of data sources for atmospheric, astrophysical and plasma modelling work. PA also has significant data users among its astrophysicists and atmospheric physicists.
UCL/PA will lead the activity defining a dictionary and semantics for atomic and molecular data storage and retrieval; will overview the construction of a modern atmospheric database (eHITRAN) in collaboration with Harvard-Smithsonian (home of HITRAN); will participate in activities associated with astrophysical data particularly when involving extremely large datasets.
Key Persons
Jonathan Tennyson Massey Professor of Physics
Chairs a IUPAC task group creating a database of water transitions, member of the HITRAN international advisory committee, member of IAEA collaborative research project on "Atomic and Molecular Data for Plasma Modelling". His group maintain a web based archive of molecular linelists for key molecules for high temperature astrophysical apprlications.
Dugan Witherick Postdoctoral Research Associate
Expert on eLearning and eScience.and associated software developments.

2.3.3.2 UCL/MSSL

is a leading Space Science research institute with skills in scientific data acquisition, processing and distribution along with a broad range of relevant software skills. MSSL has about 25 IT staff and extensive computing facilities, has an annual budget of more than £7M and a total staff of 160. UCL/MSSL has been a major partner in the UK Astrogrid program during the past seven years. Astrogrid activities at MSSL have included:

- Adaption of a range of scientific algorithms for use as Astrogrid Tools. Mainly IDL-based, these include specialized solar physics tools e.g. Movie Maker, image overlays, magnetic field extrapolation, helicity computation, coronal loop recognition, event time cross matching
- Development of: Astrogrid Data Set Access (DSA) to address relational databases; Astrogrid Registry system; Plastic-based tool for communication between desktop GUIs; Simple Time Access Protocol (STAP) for VO data access with special reference to the US VSO and CDAW systems

The computing staff is skilled in a broad range of software systems including ADA, C, C++, IDL, JAVA and Pearl together with a number of specialist systems for control and processing on-board spacecraft.

Key persons
J.L. Culhane, FRS; Professor of Physics. Very experienced solar physics; expert on applications of data bases
G. Del Zanna; Advanced Research Fellow, Chianti data base availability; WP 11
K. Benson; Senior Software Developer; Extensive Astrogrid experience.

2.3.4 Open University (OU)

The Open University hosts one of the UK's largest astronomy, space and planetary science research groups with over 100 academic and research staff based in its Centre for Earth, Planetary, Space and Astronomy Research (CEPSAR). The staff playing a leading role in several of Europe's and NASA's space missions and as such are a major user of atomic and molecular data. In 2004 the atomic, molecular and plasma (AMP) physics research group was established to support CEPSAR based research through a fundamental research programme to generate atomic and molecular data. Led by Professor N J Mason the AMP group studies the interaction of electron interactions with atom and molecules group and photoabsorption cross sections of molecular systems both in the gas and condensed phase. Such data is currently being compiled into data repositories for use in astrochemistry and plasma processing models, the latter in collaboration with Quantemol, a spin off company with one of the other partners (UCL). The OU AMP group is recognised as one of the international experts in the assessment of both electron interaction databases and photoabsorption
cross section data.

Key Persons:

N J Mason, Professor of Molecular Physics He is a leading member of the Framework VII I3 programme for planetary Science 'Europlanet' which includes the development of the Integrated Data Information Service (IDIS). IDIS will provide a comprehensive data base for planetary and
space science including spectroscopic and collisional cross section data. Within this I3 the OU will provide access to its experimental facilities to measure further data. The OU AMP Research group leads two major EU research collaborations, the Electron Induced Processing At the Molecular
Level (EIPAM) network, the Electron and Positron Induced Chemistry (EPIC) - a Framework VI Initial training Network and is a co-chair of the Electron Controlled Chemical Lithography Network (ECCL) programmes that have brought together the EU's leading research groups in electron-molecule interactions to coordinate ERA research in electron induced chemistry. The AMP group also leads the EU Japan research network on plasma processing bringing together academic researchers with data users in the plasma and semiconductor industries. The AMP group has led an EU wide programme in the study of atomic and molecular processes involved in radiation damage and the study of the effect of ionizing radiation of biomaterial (including DNA and other cellular material). The AMP group is also a member of the UK and EU ITER Fusion research programmes, perhaps the largest user of atomic and molecular data in the ERA.

Dr J Gorfinkiel: Lecturer specialising in electron-molecule interactions

Dr D Jaksch; Postdoctoral research developing electron-molecule collision

database

Role in Project: The OU will lead NA2 the dissemination and training programmes exploiting its well established links with atomic and molecular user communities (astrochemistry, plasma and semiconductor industry, ITER fusion programme and radiation sciences) to ensure that the VAMDC e-infrastructure has the widest consultation with its client base. The OU will also integrate its data depositories into the VAMDC databases (SA1), including the molecular solids physical properties databases (JRA1) and will be involved in the development of publishing tools (JRA2) and query protocols (JRA3), whilst contributing to the quality assurance of data and resources (SA2).

2.3.5 Universitaet Wien (UNIVIE)

The spectroscopic team at the Institute for Astronomy of the University of Vienna has its roots in research activities on chemically peculiar stars. It was the need for a large and user friendly atomic database, which triggered the creation and development of VALD, at that time an acronym for Vienna Atomic Line Database, to a very efficient tool for high precise abundance determinations and model atmosphere computations. The success of VALD is illustrated by the fact that other teams outside of Austria have taken over key roles for various aspects, which frequently are in the responsibility of personnel educated or strongly linked to Vienna.

Key persons:

Werner W. Weiss, professor, leader of the SAPS (Stellar Atmospheres and Pulsating Stars) group. More information can be found at http://ams.astro.univie.ac.at.

Christian Stuetz, now staff member of the University Computer Centre (ZID), VALD administrator.

Theresa Lueftinger, Nicole Nesvacil, Luca Fossati, Richard Neuteufel, are deeply involved in modelling stellar atmospheres of B to G stars at or close to the MS, abundance and stratification analyses, magnetic field determinations, Doppler and Magnetic Doppler Imaging. They are prime contacts for testing of VALD and for quality assessments, in particular for new software features and line lists.

Role in Project:

UW-A will contribute in SA1, providing service activities in support of the deployment and integration of the VALD data resources. They will contribute to JRA2, developing extensions to the publishing tools required by this large data resource.

2.3.6 Uppsala Universitaet (UU)

The Department of Physics and Astronomy of Uppsala University is one of the world-leading centres in stellar physics, galactic chemical evolution and planetary research. The emphasis is

made on theoretical and observations studies of radiation-matter interaction in the outer stellar envelopes and stellar environment, dynamics and microphysics including chemistry, phase transitions, deviations from equilibrium etc. Targets of interests are chemically peculiar and active late-type
stars, young stars with protoplanetary disks, stars hosting planets and stars in late stages of evolution. Methods developed or advanced at UU are spectral synthesis including NLTE, Doppler Imaging, 1D opacity sampling atmosphere modelling and 3D radiative hydrodynamic simulations. All of the above relies heavily on the availability of accurate and complete atomic and molecular data and thus UU today is the main driving force behind VALD - the major collection of AM data
for cool and intermediate temperatures and low/intermediate densities. UU is also carrying out ab intio calculations of collisional effects on line shapes, dust particle formation and growth and dust surface chemistry.

Key Persons:

Nikolai Piskunov: professor
Expertise: high-resolution stelar spectroscopy, spectral synthesis in 1D and 3D, stellar atmospheres, atomic and molecular data, partition functions and molecular equilibrium, radiative transfer in the
presence of magnetic fields.

Beng Edvardsson: assistant professor
Expertise: high-resolution stelar spectroscopy, spectral synthesis in 1D, stellar atmospheres, atomic and molecular data.

Kjell Ericsson: assistant professor
Expertise: high-resolution stelar spectroscopy, spectral synthesis in 1D, stellar atmospheres, atomic and molecular data.

Paul Barklem: researcher
Expertise: spectral line formation, collisional cross-section calculations, NLTE, spectral synthesis, atomic and molecular data, partition functions and molecular equilibrium.

Ulrike Heiter: researcher
Expertise: high-resolution stelar spectroscopy, abundance analysis, stellar atmospheres, atomic and molecular data, spectral synthesis in NLTE.

Andreas Korn: research assistant
Expertise: high-resolution stelar spectroscopy, spectral synthesis in NLTE, stellar atmospheres, atomic and molecular data.

Oleg Kochukhov: research assistant
Expertise: high-resolution stelar spectroscopy, spectral synthesis in NLTE, stellar atmospheres, atomic and molecular data, Doppler Imaging, asteroseismology.

2.3.7 Universitaet zu Koeln (KOLN)

The Cologne group of laboratory astrophysics has been founded by Gisbert Winnewisser and is lead by Stephan Schlemmer. The laboratory group concentrates on the molecular physics of species relevant for astrophysics. The laboratory group is situated in an astrophysics institute with three astronomy groups, involved in Herschel and SOFIA instrumentation and observations. The current focus of the laboratory group lies on high-resolution spectroscopy in the Infrared (2 – 20 µm) and Far-Infrared (100 µm – 1 cm) wavelength ranges. Other foci concern ion-molecule reactions in cold ion traps, the preparation of transient species like radicals and ions in cells, discharges and supersonic jets.

Detailed information on the group activities and equipment can be found at *http://www.astro.uni-koeln.de/node/119*.

Based on the main scientific expertise of the Cologne group the Cologne Database for Molecular Spectroscopy (CDMS) has been built over the last couple of years with significant support inside a national collaborative research effort (SFB494). Meanwhile it contains ~ 450 species, ~ 40,000 experimental lines and more than 800,000 predicted lines with very high accuracy. To date CDMS turned into the leading database in the sub-mm wavelength regime.

Recent laboratory work in the Cologne group includes high resolution spectra on complex organic molecules, e.g. dimethyl ether, with a focus on excited states which are missing in the databases, rotational and ro-vibrational spectroscopy of H_2D^+, and other cations, the IR and FIR spectroscopy of carbon chain molecules which are one of the main targets to be found by Herschel observations via their low lying vibrations. The constant development of state-of-the-art radiation sources ensures a leading role in spectroscopy. Superlattice devices fabricated by one of our collaborators, D. Paveliev, are used to generate sub-mm waves at highest frequencies and a home-made cw-OPO laser system is currently used for high resolution IR spectroscopy of molecular ions. Molecular Physics taught by the Cologne group is one of the seven main topics chosen by physics students at the university. Several young students enter the group every year.
Key Persons
Stephan Schlemmer, Professor
Expertise: physicist, head of laboratory group, molecular spectroscopy, reaction dynamics, ion chemistry, trapping, jets
Thomas Giesen, Researcher
Expertise: physicist, molecular spectroscopy, carbon chemistry, jets
Frank Lewen, Researcher
Expertise: physicist, molecular spectroscopy, THz radiation (generation & detection)
Holger Müller, Researcher
Expertise: chemist, molecular spectroscopy, leading CDMS scientist
Jürgen Stutzki, Professor
Expertise: physicist and astronomer, head of astronomy group, PI on several sub-mm astronomy projects
Peter Schilke, Senior Researcher
Expertise: astronomer, PI on several sub-mm astronomy projects

2.3.8 Istituto Nazionale di Astrofisica (INAF)

2.3.8.1 Osservatorio Astronomico di Cagliari (OAC)

OAC is one of the Research Structures of the Istituto Nazionale di Astrofisica (INAF). A variety of astronomical and technological research activities are pursued at OAC. It homes one of the world-leading groups of pulsar research, an extragalactic radioastronomy group, an astrochemistry group. It has been involved in several instrumental projects, such as the TNG Italian optical telescope at the Canary Islands, the FLAMES instrument now operating at UT2 of the ESO VLT. It is now involved in building the new 64m Sardinia Radio Telescope (http://www.srt.inaf.it), and two HPC clusters which will be nodes of the upcoming distributed supercomputing facility Cybersar (http://www.cybersar.com).
The astrochemistry group at INAF-OAC studies the photophysics of large molecules in space through a combined theoretical/modelling + multi-wavelength observational approach. In collaboration with Dr C. Joblin at CESR Toulouse, in 2003 the astrochemistry group started to build a database of the computed spectral properties of a large number of polycyclic aromatic hydrocarbons, currently available at http://astrochemistry.ca.astro.it/database. This group is recognised as one of the international leaders in the field of interstellar PAHs.
Key Persons:
Giacomo Mulas, staff astronomer
Expertise: astronomical and theoretical spectroscopy, headed the development of the data reduction software for the FLAMES–UVES, molecular modelling in astronomical environments, quantum chemistry, supercomputing.
Giuliano Malloci, post-doc fellow
Expertise: molecular modelling in astronomical environments, quantum chemistry, supercomputing, PAH spectral database.
Role in VAMDC project: definition of database structure for large molecules, related XML schemas, connected specifications (in WP7); creation of automated tools to facilitate the ingestion of current and future data of our PAHs database in VAMDC, enabling (almost) automatic update and synchronisation and foreseeing the inclusion of PAH data from other sources, such as NASA Ames (in WP8); actual deployment of our PAHs database as a VAMDC node (in WP4); maintenance and monitoring of our VAMDC node (in WP5).

2.3.8.2 Osservatorio Astrofisico di Catania (OACT)

OACT is one of the Research Structures of the Istituto Nazionale di Astrofisica (INAF). Research interests at OACT include: multi-wavelength researches on the Sun, Solar System, Stars, Interstellar Medium, External Galaxies, Cosmology; Astrobiology and search for extraterrestrial planets; Laboratory on energetic processing of solid materials; technological activities on detectors and focal-plane instruments for telescopes; high performance calculations (including GRID-computing). In particular the group LASP (Laboratory for Experimental Astrophysics) has been mainly devoted to experimental studies of the chemical and physical modifications induced by fast ions on targets of astrophysical relevance (frozen gases, silicates, carbonaceous materials). Among the induced effects particular relevance is given to the chemical modifications that, when targets contain carbon atoms, drive the formation of organic refractory residues and sub-oxides. The relevance those results have to the physics of solid surfaces in the Solar System has been outlined in several invited reviews. The laboratory is equipped with ion implanter (Danfysik 1080 200kV), OPTHOS VUV Lamp

(10.2 eV), High Vacuum (better than 10-7 mbar, or 7.5 10-8 torr) scattering chamber, Macro-micro FTIR Spectrophotometers (0.5-200 micrometer), UV-VIS-NIR Spectrophotometer (175-3200 nm), Confocal Raman spectrograph (macro and micro).

Key Persons:

Giuseppe Leto, staff astronomer

Expertise: aastronomical and laboratory spectroscopy, supercomputing, LASP database, outreach.

Maria Elisabetta Palumbo, staff astronomer

Expertise: infrared spectroscopy, ion irradiation, UV photolysis, molecules in dense interstellar molecular clouds.

Role in VAMDC project: definition of database structure for ion– and UV–irradiated ices, related XML schemas, connected specifications (in WP7); creation of automated tools to facilitate the ingestion of current and future data of our database of laboratory measurements in VAMDC, enabling (almost) automatic update (in WP8); actual deployment of our database of laboratory measurements as a VAMDC node (in WP4); maintenance and monitoring of our VAMDC node (in WP5).

2.3.9 Queen's University Belfast (QUB)

Queen's University Belfast is celebrating its centenary as an independent degree-awarding university this year. It is the leading university in Northern Ireland and a member of the Russell Group, a grouping of twenty of the leading research-intensive universities in the UK. It has a long and illustrious reputation in atomic and molecular physics with many of the founding fathers of the subject (Massey, Bates, Dalgarno) having been members of academic staff. Research in astrophysics is undertaken in the School of Mathematics and Physics in the Centre for Theoretical Atomic, Molecular and Optical Physics and in the Astrophysics Research Cluster (ARC). The work to be undertaken at QUB will be led by Professor T J Millar, one of he world's leading astrochemists and creator and maintainer of the UMIST Database for Astrochemistry, and who leads the Molecular Astrophysics group in ARC. Refereed publications associated directly with the Database were the 2nd and 4th most highly cited papers in astrochemistry in the past decade according to the Thomson Web of Science. Professor Millar ranked number one in the list of cites per paper. Millar is Chair of the International Board of the James Clerk Maxwell telescope in Hawaii and Chairman of Division VI (Interstellar Matter) of the International Astronomical Union.

Role in the Project: Professor T J Millar will collaborate to the deployment of his database in the VAMDC e-infrastructure. He will be a member of the SPC.

2.3.10 Astronomska opservatorija (AOB)

AOB is a multidisciplinary institution covering the Atomic physics in particular theoretical determination of Stark broadening parameters of non hydrogenic atoms and ions, where together with the partners in LERMA (S. Sahal Brechot), has one of the leading position in Europe; physics and spectroscopy of Active Galactic Nuclei; stellar physics, close binary systems; solar physics; asteroids, minor bodies of the solar system; astrometry, and dynamical astronomy. AOB is an independent institution financed mainly through the projects of

Ministry of Science and Technological Development of R. Serbia.
The first attempts to start the organization of a database started in 2000 and in 2008 started the project of the Serbian virtual observatory, with the objective that it enter in the future in the European virtual observatory. As a beginning, started in 2000 the work to organize Stark broadening data obtained during the more than 30 years of collaboration with LERMA (S. Sahal-Brechot). In 2005 started the collaboration with the database Stark-B at Paris observatory with the objective to obtain two mirrors, one in Belgrade and one in Paris.

Key Persons:
M.S. Dimitrijevic (AOB) Senior Researcher
Expertise:Stark broadening data, Atomic Physics, Influence of Collisional processes on stellar and laboratory spectra, Serbian coordinator of the Serbian-Bulgarian project at both Academies "Development and application of astronomical databases, member of the team of the project "Serbian
Virtual Observatory.
Role in VAMDC project: Coordinator of the project (from AOB), connection to the users of Stark broadening data, testing and producing Stark broadening data. Quality assurance.
L. Ch. Popovic (AOB) Senior Researcher
Expertise: Stark broadening theory, spectra of AGN, stellar spectra, databases
Role in VAMDC project: calculation and testing of Stark broadening data, AOB mirror site. Quality assurance, Belgrade Cluster
D. Jevremovic (AOB) Researcher
Expertise: Stellar spectroscopy, modelisation of stellar spectra, stellar atmospheres codes (PHOENIX), Leader of the project "Serbian Virtual Observatory.
Role in VAMDC project: connection to users in stellar spectra domain and stellar atmospheres code domain, connection to Serbian Virtual Observatory, AOB mirror site, Belgrade Cluster
Z. Simic (AOB) Researcher
Expertise: Determination and testing of Stark broadening data, Atomic Physics
Role in VAMDC project: testing and calculation of Stark broadening data, AOB mirror site.
E. Bon (AOB) PhD student
Expertise: Databases development and management, Spectra of Galaxies and AGN
Role in VAMDC project: Belgrade mirror site, Belgrade cluster
N. Milovanovic (AOB) PhD student
Expertise: Determination and testing of Stark broadening data, Atomic Physics, databases development and management
Role in VAMDC project: testing and calculation of Stark broadening data, AOB mirror site, Belgrade cluster.
A. Kovacevic, Belgrade Mathematical Faculty, AOB, Docent
Expertise: Determination and testing of Stark broadening data, Databases
Role in VAMDC project: testing and calculation of Stark broadening data, AOB mirror site, Belgrade Cluster.

2.3.11 Institute for Spectroscopy RAS (ISRAN)

Institute for Spectroscopy RAS (ISRAN) is an Establishment of the Russian Academy of Sciences. Director of the Institute - Prof. E.A.Vinogradov, Corresponding member of the Russian Academy of Sciences The Institute carries out spectral investigations of atoms,

multicharged ions, plasma, molecules (both the simplest molecules in gas phase and complex organic ones in solid matrices), liquids, crystals and films, multilayer thin structures, superlattices, quantum wells, other nanostructures, high temperature superconductors, solid state surfaces, biological objects. The studied spectra cover a wide spectral range from X-rays to microwaves. The Institute has a series of unique spectral instruments and setups: 1) instruments having high spectral resolution up to 10-6cm-1, time resolution up to 3x10-14s, and local resolution up to 5 nm, 2) methods and instruments for ultrasensitive detection of atom traces (isotopes) and molecules in gaseous, liquid and solid samples with detection limit up to several femtograms (10-15gram) in a sample, 3) methods and instruments for investigation of ultra thin films (down to monolayers) on the surface of metals and dielectrics and for new surface physics data.

Scientific structure of ISRAN includes 9 scientific departments. One of them is Atomic Spectroscopy Department, chief of department - Prof. A.N.Ryabtsev. The purpose of the department is the receiving of experimental and theoretical data about energy structures of atoms and ions which are necessary for astrophysics, for works on controlled thermo-nuclear synthesis, for the creation of vacuum ultra-violet and X-ray lasers, and also for the development of spectral diagnostics of high temperature plasma.

For 40 years ISRAN is involved in laboratory analysis of the atomic and ionic spectra throughout the Periodic Table from the light elements such as boron to heavy elements of palladium group. More than 30000 spectral lines were identified in about 290 atomic and ionic spectra. The work is based on a high resolution spectroscopic equipment and on the theoretical calculations of atomic spectra using a variety of theoretical approaches (Hartree – Fock, Dirac – Fock, orthogonal operator technique and others). A Database of Bibliography on Atomic Spectra (BIBL) was created and maintained. It is accessible on line from the site http://das101.isan.troitsk.ru/bibl.htm The topics covered by BIBL are:

- Spectra of atoms and atomic ions: ionization potentials, line classification, energy levels, wavelengths, hyperfine structure, isotopic effects, broadening and shifts of spectral lines, the Stark and Zeeman effects, plasma diagnostics, astrophysical spectra, theory of atomic spectra, radiation and autoionization rates, oscillator strengths, QED and relativistic effects in atoms and ions, atomic-spectroscopy tests of the fundamental principles, spectral sources, techniques of spectral measurements.
- Cross sections of the collision processes: excitation and ionization by electrons and photons, multiphoton processes, Auger decay, ion-electron recombination. To less extent - charge exchange, excitation and ionization in collisions with heavy particles - if any new data related to the atomic structure are obtained in these publications.

The bibliography related to experimental and theoretical papers on identification and prediction of atomic and ionic structure should be complete from 1983, the year of the last issue of NBS Special Publication "Bibliography on Atomic Energy Levels and Spectra", but the experimental spectrum analysis can be traced back to about 1970. On the other topics, it is systematically maintained since 1989. For the last decade ISRAN is involved in the analysis of ion spectra of the rare earth elements, production and critical evaluation of atomic data (energy levels, wavelengths, transition probabilities and magnetic g-factors) for Vienna Atomic Line Database (VALD).

Key Contacts:

Prof. A.N.Ryabtsev, head of Department of Atomic Spectroscopy ISRAN

Role: Atomic data production, critical evaluation of published atomic data, bibliography database maintenance.

Dr. R.R.Kildiyarova, senior scientific worker, ISRAN

Role: Atomic data production, critical evaluation of published atomic data, preparation of the data for incorporation into VALD

2.3.12 Russian Federal Nuclear Centre – All Russian Institute of Technical Physics (RFNC-VNIITF)

Russian Federal Nuclear Centre All-Russian Institute of Technical Physics (RFNC VNIITF) is a multidisciplinary national scientific centre of the Russian Federation running research and development programs in the domain of high-energy-density physics (HEDP) and related fields of physics, computer science, material science, and technology. Appropriate modeling of EUV and x-ray emission and absorption spectra of matter under extreme conditions of hot laboratory and astrophysical plasmas is an inherent feature of the HEDP research and, in turn, implies realistic description of atomic-structure and spectral properties of various multielectron ions. The latter activities are being run at the institute for more than two decades and involve spectroscopic-data calculations for multielectron ions and elaboration of atomic databases; development of theoretical models to calculate detailed Stark-broadened lineshapes; and development of theoretical models to calculate opacities of the multielectron-ion plasmas utilizing both the detailed and statistically averaged description of the bound-bound and bound-free transitions. The spectroscopic constituent of the effort, in particular, resulted in the creation of the Spectr-W^3 information-reference system (http://spectr-w3.snz.ru) providing free round-the-clock access to the Spectr-W^3 factual atomic database and presenting experimental, calculated, and compiled data on ionization potentials, energy levels, wavelengths, radiation transition probabilities and oscillator strengths, and also parameters of analytical approximations of electron-collisional cross-sections and rates for atoms and ions. The Spectr-W^3 project is being implemented under the long-term collaboration with the high-level experts of the Joint Institute for High Temperatures of Russian Academy of Sciences (JIHT RAS) and partial support of International Science and Technology Centre (ISTC, www.istc.ru). To date, Spectr-W^3 atomic database is still the largest factual database in the world, containing the information on spectral properties of multicharged ions (about 450,000 records).

Key Persons.

P.A. Loboda, Dr. of Science, Principal scientist.

Expertise: atomic physics, lineshape theory, and spectroscopy of hot dense plasmas. Leader of the Spectr-W^3 project.

Role in VAMDC project: coordinator of the project (from RFNC VNIITF), connection to the users of the Spectr-W^3 database, testing and calculation of atomic data, development of algorithms for interfaces to represent the Spectr-W^3 data in line with the common VAMDC standards for data inquiry and output, interoperability and publication tools. SAs, JRA1, JRA2.

I.Yu. Skobelev, Dr. of Science, Leading scientist.

Expertise: atomic physics, spectroscopy of hot dense plasmas.

Role in VAMDC project: data assessment, quality assurance, testing and calculation of atomic data, interoperability issues. SA1, JRA1.

S.V. Gagarin, Head of laboratory. Expertise: multidisciplinary computer science.

Role in VAMDC project: Development of XML schemas and user-interface utilities to represent the Spectr-W^3 data in line with the common VAMDC standards, interoperability, publication, new mining and integration tools. SA1, JRAs.

S.V. Morozov, workgroup leader.

Expertise: database developments and programming. Development of the user-interface utilities, Spectr-W^3 database maintenance and upgrade. SA2, JRA2, JRA3.

2.3.13 Institute of Atmospheric Optics (IAO)

IAO is the leading institute of the Russian Academy of Sciences (RAS) in the fields of atmospheric optics, ecological monitoring and climate changing.
One team from this institute involved into the project deals with the modeling of high resolution spectra of the molecules of atmospheric and astrophysical interests. This team in collaboration with LPMAA (CNRS, France) has elaborated Carbon Dioxide Spectroscopic Databank (CDSD) and in collaboration with GSMA (CNRS, France) does Spectroscopic Databank on Ozone Molecule. On the basis of these databanks it has elaborated two Internet accessible information systems.
Anothere team is specialized in Information system Management.

Key Persons:

V.I. Perevalov is the head of the Laboratory of Theoretical Spectroscopy (DR).
Expertise: scientific leader in the modeling of high resolution spectra of molecules of the atmospheric and astrophysics interests and in the elaboration of the database of molecular spectral line parameters.
Role in VAMDC project: coordinator of IAO node, Leader of team 1, molecular expert, CDSD database, NA2, JRA2.

A.Z. Fazliev, Senior Researcher (DR).
Expertise: Information system management.
Role in VAMDC project: Leader of Team 2, Distributed information system W@DIS, NA2, JRA2

A.I. Privesetsev, Researcher (team 2)
Expertise: Semantic metadata management.
Role in VAMDC project: implementation of software processing metadata, JRA2.

A.V. Kozodoev, Researcher (team 2)
Expertise: Database management.
Role in VAMDC project: implementation of software processing data, JRA2.

Y.L. Babikov, Research engineer (team1)
Expertise: Information system management.
Role in VAMDC project: CDSD and S&MPO databases, NA2, JRA2.

S.N. Mikhailenko, Senior Researcher (DR), (team 1)
Expertise: Molecular expert.
Role in VAMDC project: S&MPO database, JRA2.

S.A. Tashkun, Senior Researcher (DR), (team 1)
Expertise: Molecular expert.
Role in VAMDC project: CDSD database, JRA2.

2.3.14 Corporacion Parque Tecnologico de Merida (CPTM)

Two institutions will take part in the Venezuelan node:

2.3.14.1 Laboratory of Computational Physics

(LCP, http://www.ivic.ve/fisica/?mod=computacion.php), Physics Center, Venezuelan Institute for Scientific Research (IVIC), Caracas, and

2.3.14.2 National Center for Scientific Computing

Universidad de Los Andes (CeCalCULA, http://www.cecalc.ula.ve/), Merida.

The LCP consists of two senior research fellows and 5 postgraduate students while CeCalCULA has four senior and two junior research fellows, two engineers and six postgraduate students. The LCP has had a long time involvement in the computation of atomic data for astrophysical applications and in the development of atomic databases. These research lines have included collaborations at the international level with both American and European groups. CeCalCULA is, together with Mexico and Brazil, one of the operational nodes of EELA-2 (E-science grid facility for Europe and Latin America, http://www.eu-eela.eu/), and the main promoter in Venezuela and the Andean region of e-science initiatives and grid computing, especially in bioinformatics (see http://portal-bio.ula.ve). CeCalCULA has a long-term experience in the organization of EELA workshops and summer schools.

Claudio Mendoza (CPTM), Professor
Expertise: Expert in atomic physics, grid technology, database management
Role in VAMDC project: Deployment of TIPTOPbase, Opserver, XSTAR (SA1, SA2)
L. Nunez (IVIC), Professor
Expertise: Expert in grid technology, database management
Role in VAMDC project: Deployment of TIPTOPbase, Opserver, XSTAR (SA1, SA2)

2.3.15 Institute of Astronomy RAS (INASAN)

Since 1995 INASAN is responsible for maintaining and updating the content of the VALD. This task includes the search and critical evaluation of the new data, quality control and recommendations for the users via the so-called ranking list for various parameters stored in the VALD. Ranks are established based on the techniques used to derive atomic and molecular parameters, quality estimates given by the data producers and the comparison with the results of spectral analysis of astrophysical standards such as the Sun, Vega, Procyon etc.

Key Person
Dr. T.A.Ryabchikova, leading scientist
Expertise: The main responsibility of INASAN is the verification of quality and completeness of the data in atomic and molecular lines databases for various astrophysical applications and the inter-comparison between overlapping the data in different databases. High-quality spectra of astrophysical objects are used for these purposes and the methodology is well developed and routinely used for the content of the Vienna Atomic Line Database (VALD).
Role in VAMDC project: Search for the new data. Contacts with data producers. Cross-comparison of the new data using spectra of the astrophysical objects. Preparation of the new data for ingestion into VALD. Final recommendations for the users (SA2), (NA2)

2.4 Management of Risk

NA WPs: Risk assessment

The risks related to the VAMDC project that have been identified are stored in a Risk Register, assessed and classified using the fairly standard following scheme:

- likelihood of occurrence (1 = very unlikely to 4= highly likely)
- likely impact (1 = minimal impact, 4 = disastrous)

The product of (likelihood of occurrence * likely impact) provides the risk factor (ranging from 1 (minimal risk) to 16 (extremely high risk).

Risks with a highest risk factor are the ones on which attention should be mostly focused. For each identified risk a mitigation action is provided. The Risk Register will be maintained throughout the project, in the sense that it is periodically verified, to add new risks or to update the risk factors: if the mitigation actions are performed successfully, risks may be retired from the Register. Risks associated with NA programme have been assessed as follows:

Risk	**Consequences**	**Mitigation Action**
Risk NA-R1: **Failure to reach agreement on the policies and strategies for the project** Likelihood of occurrence=2 Impact=3 **Risk Factor = 6**	Discussions within the Board and the Executive Project Team will not lead to a shared vision of the project's policies and strategies, hampering the possibility of a unified view of the project.	Different technical solutions may be pursued, with a close eye on allowing interoperability between them. This solution has a higher cost in terms of person-power.
Risk NA-R2: **Failure to achieve cross-activity coordination** Likelihood of occurrence=2 Impact=3 **Risk Factor = 6**	Failure to achieve consensus within the governing teams of the project, or limited collaboration may hampering the possibility of achieving a set of results sharing the same technical solutions. This would lead to possible misuse or duplication of efforts	Special care will be taken to ensure that the NA1,2 and SAs/JRAs activities work in good agreement, since SAs/JRAs depend on NA1,2 decisions: this will be enforced by periodic one-one meetings via teleconference. As for other work-packages, special meetings via teleconference for the VPB and EPT will be set whenever a problem between/among work-packages arises.
Risk NA-R3: **Lack of convergence between the scope of training and the real needs of the communities**	If the scope of the training activities is too vague or too general, not in line with the real needs of the users and developers communities, there will be few	VAMDC partners are involved in producing, collecting, diffusing AM data, as well as in technological developments. Most partners have a long

Likelihood of occurrence=1 Impact=3 **Risk Factor = 3**	attendances to the training events and their impact will be limited	experience of organizing conferences and tutorials for AM data. Among all the boards and committees, it shall be easy to identify the needs and requirements for such events so there is little risk that the scope of these workshops/tutorials is not adequate.

The identified risks for the Network Activities of the VAMDC project have risk factors up to 6, with mitigation actions in all cases that would limit the impact of such risks. **The overall level of risk of the VAMDC Network Activities is low.**

SA List of risks and mitigation actions

Risk	**Consequences**	**Mitigation Action**
Risk SA-R1: **Not enough human resources to perform the Services Activities** Likelihood of occurrence=2 Impact=3 **Risk Factor = 6**	Some of the tasks within these Service Activities could require more person-power then currently planned. This would lead to a overall delay in deployment of resources. The output of the VAMDC services activities would be limited by the funded and contributed person-power.	Services Activities will need to be prioritized by decision of the VPB and technical advice from the EPT, to make sure resources are directed first to what is more important. If necessary, partners involved in Service Activities could seek through their own funding to increase their contributed person-power to be able to cope with the extra work-load.
Risk SA-R2: **Lack of convergence between the scope of the Service Activities and the real needs of the communities** Likelihood of occurrence=2 Impact=3 **Risk Factor = 6**	Groups in charge of Service Activities may opt to choose technical solutions which are in contrast with the needs or experiences of the user communities.	The plan for the deployment of the Service Activities will need to be clearly defined and agreed by the Board under technical advice from the EPT, where a match between user needs and services provided will be made. Bottom up information from users will be provided through the CTC and Task 3 of WP2
Risk SA-R3: **Lack of interest of the Scientific Community for deploying their resources in the VAMDC infrastructure** Likelihood of occurrence=2 Impact=4	If the Scientific Community (both EU and non-EU) is not interested in porting their resources to the VAMDC e-infrastructure, the VAMDC project will loose a big fraction of its interest.	Through the SAB and the EPT the VAMDC project will make sure to stay close to the user communities. Moreover through the dissemination and training in EU and non-EU countries, the VAMDC project informs, encourages and trains new users.

Risk Factor = 8		The partnership with non-EU countries is crucial to the future acceptance of the VAMDC platform at a wide world level.

The identified risks for the Services Activities of the VAMDC project have risk factors up to 8, with mitigation actions in all cases that would limit the impact of such risks. The overall level of risk of the VAMDC Services Activities is low.

List of risks and mitigation actions

Risk	Consequences	Mitigation Action
Risk JRA-R1: Failure to reach coordination in the development of standards Likelihood of occurrence=3 Impact=3 **Risk Factor = 6**	Service interfaces deployed at nodes are not interoperable. Standards cannot be implemented at some nodes.	Engage data publishers during development of standards to check feasibility. During standards definition, make low-cost prototypes of the services and deploy them for tests.
Risk JRA-R2: VAMDC standards duplicate work in existing user communities (including external developments made during VAMDC project) Likelihood of occurrence=3 Impact=2 **Risk Factor = 6**	Wasted effort; possible extra development to adapt VAMDC infrastructure to work with external software.	Send VAMDC delegates to external standards bodies (e.g. IVOA, EuroPlanet).
Risk JRA-R3: registry-mining protocol defeated by incomplete/inaccurate metadata Likelihood of occurrence=3 Impact=2 **Risk Factor = 6**	Users fail to discover and use all appropriate resources. Users waste time with inappropriate resources.	Ensure that data publishers understand the metadata schemata; provide extensive documentation. Allow publishers to enter their own metadata to avoid errors in transcription; provide a good UI for this. Implement automatic checks of registry consistency and correctness that can be run frequently.
Risk JRA-R4: data-mining	These tools are under used;	Provide good documentation with

tools are complex and difficult to use Likelihood of occurrence=4 Impact=2 **Risk Factor 8**	researchers miss opportunities. Researchers misunderstand the constraints on using the tools and derive incorrect results.	many examples of use and clear statement of domain of applicability. Perform usability tests of tools with sample groups of users. Consider providing simplified UIs for common uses of the tools.

The identified risks for the Joint Research Activities of the VAMDC project have risk factors up to 8, with mitigation actions in all cases that would limit the impact of such risks. The overall level of risk of the VAMDC Joint Research Activities is low.

3. WORK PACKAGES SUMMARY

Work package list

Work package No	Work package title	Type of activity	Lead beneficiary No	Person-months	Start month	End month
WP1	MGT: Project Management	MGT	1	58	1	42
WP2	NA1: Science/Technical Coordination of the network	COORD	1 + 2	62	1	42
WP3	NA2: Dissemination and Training	COORD	4	91	3	42
WP4	SA 1: Infrastructure Deployment	OTHER	2	219	3	42
WP5	SA 2: Support to the Infrastructure	OTHER	1	158	3	42
WP6	JRA1: Interoperability	RTD	7	96	3	42
WP7	JRA2: Publishing Tools	RTD	6	65	3	42
WP8	JRA3: New mining and Integration Tools	RTD	3	72	3	42
	TOTAL			821		

3.1 Management and Networking Activities

3.1.1 Overall Strategy and General Description

The ensemble of Networking Activities (NAs) aims to foster a culture of cooperation between A&M scientists, database providers and data users throughout Europe. Three WPs are planned;

WP1 (MGT): Project Management
WP2 (NA1): Science/Technical Coordination of the network
WP3 (NA2): Dissemination and Training

WP1 is centred on Management and direction of the overall infrastructure programme and therefore is mainly concerned with the internal management of VAMDC. This includes responsibility for the finance control of the project, reporting to the EU, and formal packaging of deliverables. The second WP (NA1) provides the scientific and technical direction necessary for the operation of the VAMDC e-infrastructure developing its structures and integrating with other data services, while WP3 (NA2) provides the interface of VAMDC to the wider user community, being responsible for training and dissemination. The objectives of NA1,2 are: to coordinate the infrastructure's activities among all trans-disciplinary fields (atomic and molecular physics, users such as the astrophysics, atmospheric, fusion, ICT communities); to develop a coherent research community within the EU and to create a direct partnership to key external communities in both the Russian Federation and central and southern America via Venezuela: to link VAMDC to other international projects relevant to VAMDC; to interact with non-partner teams from other EU and non-EU countries in order to take the largest possible approach to the development of the infrastructure: to disseminate VAMDC achievements and to get feedback from data provider and users on the content and operation of VAMDC. The NAs will therefore have both a practical and a political role in defining the policies and evolution of the infrastructure.

Each Work Package is under responsibility of one partner apart from WP2 (where a co-lead is envisaged reflecting the dual role science/technical of this WP). WP1 (CNRS, the project Chair), WP2 (CNRS/CMSUC) and WP3 (OU). The WP/NA work programmes are defined by a series of preset tasks each of which have allocated partners (See Tables 1.3.c). During the initial Kick-off phase of the project (Project months 1-3) only WP1, WP2 and WP3 will be active. At the end of the Kick-off phase, WP2 produces the project detailed work program for Cycle 1 whilst WP1, WP3 provide the Project Web site for both internal circulation of information and external dissemination of the projects aims and objectives. All WPs produce regular reports of their progress. As part of the WP2/NA1 activities, the reports are assessed by the Executive Project Team. The Executive Project Team then proposes a plan for future activities to the Board.

Concertation Activities

The project will actively participate in concertation initiatives and meetings related to the e-Infrastructures and other related areas including the participation and contribution in relevant working groups established under the above initiative. The objective of the concertation activity is to optimise synergies between projects and the collective impact and value of the programme.

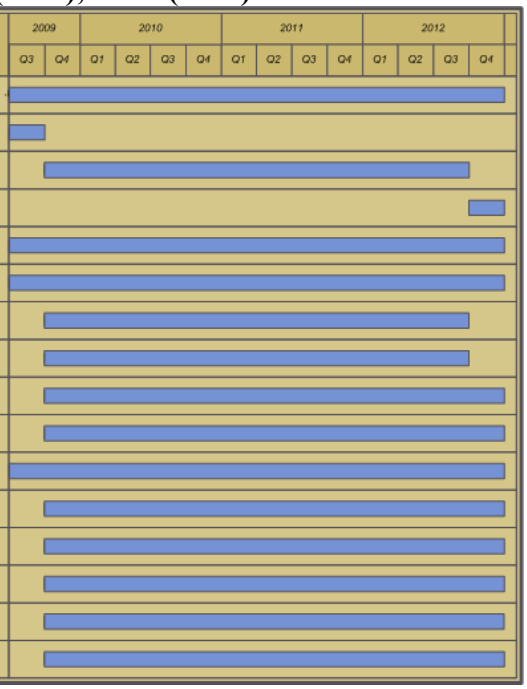
The project will also provide input for relevant European Commission initiated dissemination activities (e.g. press releases, news bulletins, brochures, success stories, posters, web-based publications, multimedia material etc). In this context the project's dissemination-messages will also reflect its broader societal and economic impact. The project's dissemination material in relation to the above goal will be regularly updated to provide the latest version of its status and achievements. This will be reflected in deliverable D1.1 (to be updated every month).

3.1.2 Timing of work packages and their components

In the following, the timing of the project overall organisation is presented as Gantt charts

Gantt Chart for WP1 (MGT), WP2 (NA1), WP3 (NA2)

ID	TASK NAME	Start	End	Start	End
1	**WP1: MANAGEMENT**	Month 1	Month 42	01/07/2009	31/12/2012
2	Task1:VAMDC Kick-Off Phase	Month 1	Month 3	01/07/2009	30/09/2009
3	Task2: Project Management	Month 3	Month 39	30/09/2009	01/10/2012
4	Task3: Termination of Project	Month 39	Month 42	01/10/2012	31/12/2012
5	**WP2: S/T Coordination**	Month 1	Month 42	01/07/2009	31/12/2012
6	Task1: Internal Technical Activities	Month 1	Month 42	01/07/2009	31/12/2012
7	Task2: Connection to External Technical Project	Month 3	Month 39	30/09/2009	30/09/2012
8	Task3: Collect user/producer specifications	Month 3	Month 39	30/09/2009	30/09/2012
9	Task4: Policies concerning Standards	Month 3	Month 42	30/09/2009	31/12/2012
10	Task5: Policies concerning publication in VAMDC	Month 3	Month 42	30/09/2009	31/12/2012
11	**WP3: Dissemination and Training**	Month 1	Month 42	01/07/2009	31/12/2012
12	Task1: Coordination	Month 3	Month 42	30/09/2009	31/12/2012
13	Task2: Organisation of Networking Events	Month 3	Month 42	30/09/2009	31/12/2012
14	Task3: Organisation Scientific Workshops	Month 3	Month 42	30/09/2009	31/12/2012
15	Task4: Organisation of Training Tutorials	Month 3	Month 42	30/09/2009	30/12/2012
16	Task5: Service&Prototype Releases	Month 3	Month 42	30/09/2009	31/12/2012



3.2 Services Activities

3.2.1 Overall Strategy and General Description

The key objective of the two Service Activities (SA1, SA2) is to provide access to an inclusive range of high quality data and applications services to the research community. The VAMDC partners represent major data producers. By integrating their existing and, importantly, future resources through the standard VAMDC infrastructure the wider community of diverse end users will gain enhanced access to this eco-system of fundamental scientific data. The SA activities will ensure the availability of these major data resources in interoperable formats, the maintenance of services allowing publications of small datasets by producer's teams, the maintenance of registries and dictionaries, the maintenance of nodes listing the needs for the various communities (in relation with other EU initiatives). These services will be delivered by use of the latest virtual observatory and grid e-science infrastructures. Extensions to the core infra-structure will be prototyped during the course of VAMDC and deployed operationally by the SA1.

To allow the project VAMDC to achieve its objectives related to the provision of services to the community of AM data producer and users, two areas of work related to Service Activities have been identified:

WP4: SA1 – Infrastructure Deployment
WP5: SA 2 - Support to the Infrastructure (led by CNRS)

SA1 (led by CMSUC) provides users with access to the assembled A&M databases. This involves implementing standard outputs for the AM databases, finding the resources by interrogating registries, using querying and pipeline tools. SA1 is supported by SA2 (led by CNRS) which provides the necessary support for operating the e-infrastructure itself, although to any user entering the e-infrastructure portal only one SA (the VADMC) will be apparent.

SA1 and SA2 will start immediately after the Kick-off phase of the project, in which the project detailed work program for Cycle 1 is defined, with different starting time for the various tasks.
SA WPs (and their sub-WPs) produce respectively mid-term and final reports one month before the end of each one-year Cycle. Their reports are assessed by the Executive Project Team which prepares respectively a mid-term and final activity report. The plan is revised at the end of Cycle 1, 2 and an updated plan is produced for the following Cycle, subject to the agreement of the Executive Project Team and approval of the Board. A final report is produced at the end of the project.

3.2.2 Timing of work packages and their components

Gantt Chart for WP4 (SA1), WP5 (SA2)

ID	TASK NAME	Start	End	Start	End
1	**WP4: Infrastructure Deployment**	Month 3	Month 42	30/09/2009	31/12/2012
2	Task1: Standard Access to AM data	Month 3	Month 42	30/09/2009	30/12/2012
3	Task2: Standard Access to Numerical Codes	Month 3	Month 42	30/09/2009	19/12/2012
4	Task3: Implementing Registries	Month 18	Month 42	22/12/2010	19/12/2012
5	Task4: Augmenting VODesktop	Month 15	Month 39	30/09/2010	30/09/2012
6	Task5: Publishing desktop software	Month 21	Month 39	30/03/2011	30/09/2012
7	Task6: Expansion of the infrastructure	Month 36	Month 39	01/07/2012	30/09/2012
8	**WP5:Support to the Infrastructure**	Month 3	Month 42	30/09/2009	31/12/2012
9	Task1: Maintenance and Monitoring	Month 3	Month 42	30/09/2009	31/12/2012
10	Task2: Grid Operation	Month 3	Month 39	30/09/2009	30/09/2012
11	Task3: Support to « users »	Month 12	Month 42	30/06/2010	30/12/2012
12	Task4: Preservation of digital data and ressources	Month 3	Month 39	30/09/2009	30/09/2012
13	Task5: QA of data and resources	Month 12	Month 39	30/06/2010	30/09/2012

4.1 Joint Research Activities

4.1.1 Overall Strategy and General Description

The objectives of the JRAs are to build the complete set of "tools" necessary to create an e-science platform for the exchange of atomic and molecular data, creating new specifications and creating/adapting/integrating new software.

The three Joint Research Activities Work Packages are defined as follows:

WP7: JRA1 Interoperability (led by UU)
WP8: JRA2 Publishing Tools (led by IAO)
WP9: JRA3 New mining and Integration Tools (led by UCL).

JRA 1 (led by UU) will define the standards necessary to build an interoperable infrastructure. It will improve and extend the current data models and XML schema in order to describe the structure of data, build dictionaries containing the most usual terminology in order to allow for easy cross-matching, design access protocols and query languages, define the structure of registries.

JRA2 (led by IAO) will provide generic tools partly using the standards developed in JRA1 in order to help producers of A&M data to publish their sets into the VAMDC infrastructure. JRA2 will develop the software that will be deployed within the VAMDC infrastructure. Some of these software will be associated to the standards developed in JRA1. The general software made available to the community will be accessible via the VAMDC technical web-site.

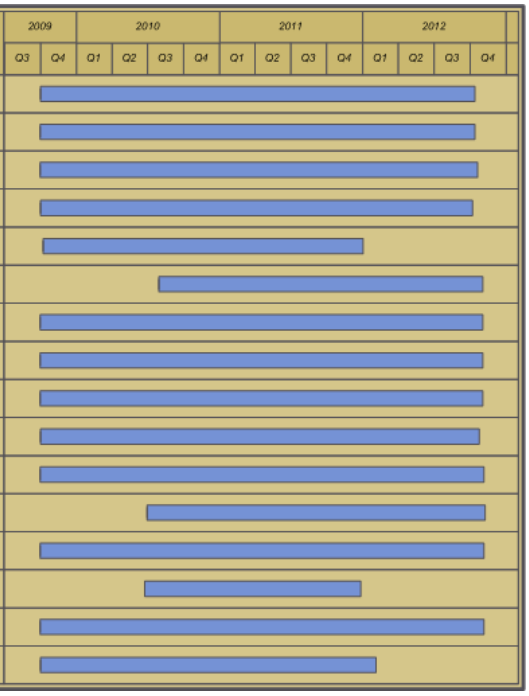
JRA3 (led by UCL) will develop new mining and integration tools allowing cross-matching or/and cross-federation of heterogeneous resources and application services wrapping complex work flows combining AM data access, manipulation, and integration into user processing chains.

Since JRAs are necessary for the development of the SA WPs , these JRAs will start immediately after the Kick-off phase of the project. Since it is essential to ensure that JRAs deliver their tools on time (or the SA deployment will be hampered) in addition to producing both mid-term and final reports, three monthly updates will be prepared and assessed by the Executive Project Team which can recommend any required changes in JRS work programme and management.

4.1.2 Timing of work packages and their components

Gantt Chart for WP6 (JRA1), WP7(JRA2), WP8(JRA3)

ID	TASK NAME	Start	End	Start	End
1	**WP4: Interoperability**	Month 3	Month 39	01/10/2009	12/10/2012
2	Task1: Data Models and XML Schema	Month 3	Month 39	30/09/2009	12/10/2012
3	Task2: Dictionnaries	Month 3	Month 39	30/09/2009	19/10/2012
4	Task3: Access Protocols/Retrieval Languages	Month 3	Month 39	01/10/2009	06/10/2012
5	Task4: Registries	Month 3	Month 30	08/10/2009	01/01/2012
6	Task5: Other Documents	Month 12	Month 39	30/07/2010	01/11/2012
7	**WP7:Publishing Tools**	Month 3	Month 39	30/09/2009	01/11/2012
8	Task1: From XML schema to DB deployment	Month 3	Month 39	30/09/2009	01/11/2012
9	Task2: Tools to build registries from content of DB	Month 3	Month 39	30/09/2009	01/11/2012
10	Task3: Interfaces to easily update dictionnaries	Month 3	Month 39	01/10/2009	23/10/2012
11	Task4: Software Libraries to generate standard outputs of DB	Month 3	Month 39	30/09/2009	04/11/2012
12	Task5: Full publishing solution	Month 15	Month 39	30/06/2010	07/11/2012
13	**WP8: Mining and Integration Tools**	Month 3	Month 39	30/09/2009	04/11/2012
14	Task1: Registry Queries	Month 12	Month 30	24/06/2010	26/12/2011
15	Task2: Tools for Manipulation of data	Month 3	Month 39	30/09/2009	04/11/2012
16	Task3: Advanced Data Mining Services	Month 3	Month 39	01/10/2009	03/02/2012



4. SUMMARY OF DELIVERABLES

List of Deliverables – to be submitted for review to EC

MGT & NA Deliverables List

Del. no.	Deliverable name	WP no.	Lead beneficiary	*Estimated indicative person-months*	Nature	Dissemination level	Delivery date
D1.1	VAMDC Website	1	CNRS	1	O	PU	2
D1.2	VAMDC Project Plan	1	CNRS	1	R	PU	3
D2.1	Science/Technical Plan	2	CMSUC/CNRS	2	R	PU	3
D3.1	Dissemination/Training Plan	3	OU	2	R	PU	3
D2.2	Science/Technical Report 1	2	CMSUC/CNRS	12	R	PU	10
D3.2	Dissemination/Training Report 1	3	OU	7	R	PU	10
D1.3	Revised Annual VAMDC Project Plan 1	1	CNRS	9	R	PU	10
D3.3	Level 1 Service Prototype	3	CMSUC/UU	12	O	RE	10
D3.4	Annual Project Meeting 1	3	OU	4	O	PU	12
D1.4	VAMDC Budget & Review Report to EU 1	1	CNRS	9	R	CO	12

D2.3	Science/Technical Report 2	2	CMSUC/CNRS	18	R	PU	22
D3.5	Dissemination/Training Report 2	3	OU	7	R	PU	22
D1.5	Revised Annual VAMDC Project Plan 2	1	CNRS	9	R	PU	22
D3.6	Level 2 Service Prototype	3	CMSUC/UU	12	O	RE	22
D3.7	Annual Project Meeting 2	3	CMSUC	4	O	PU	24
D1.6	VAMDC Budget & Review Report to EU 2	1	CNRS	9	R	CO	24
D2.4	Science/Technical Report 3	2	CMSUC/CNRS	18	R	PU	34
D3.8	Dissemination/Training Report 3	3	OU	7	R	PU	34
D1.7	Revised Annual VAMDC Project Plan 3	1	CNRS	9	R	PU	34
D3.9	Level 3 Service Prototype	3	CMSUC/UU	13	O	PU	34
D3.10	Annual Project Meeting 3	3	UNIVIE	4	O	PU	36
D1.8	VAMDC Budget & Review Report to EU 3	1	CNRS	9	R	CO	36
D3.11	VAMDC Service Release	3	CMSUC/UU	12	O	PU	40
D2.5	Final Science/Training Report	2	CMSUC/CNRS	12	R	PU	41
D3.12	Final Annual Meeting	3	CNRS	4	O	PU	42
D3.13	Final Dissemination/Training Report	3	OU	3	R	PU	42
D1.9	Final Review and Budget Report of VAMDC to EU	1	CNRS	2	R	CO	42

SA Deliverables List

Del. no.	**Deliverable name**	**WP no.**	**Lead bene-ficiary**	***Estimated indicative person-months***	**Nature**	**Dissemination level**	**Delivery date**
D4.1	Infrastructure Deployment Plan	4	CMSUC	9	R	PU	3
D5.1	Service Support Plan	5	CNRS	8	R	PU	3
D4.2	Infrastructure Deployment Report 1	4	CMSUC	40	R	PU	10
D5.2	Service Support Report 1	5	CNRS	30	R	PU	10
D4.3	Infrastructure Deployment Report 2	4	CMSUC	60	R	PU	22
D5.3	Service Support Report 2	5	CNRS	50	R	PU	22

D4.4	Infrastructure Deployment Report 3	4	CMSUC	80	R	PU	34
D5.4	Service Support Report 3	5	CNRS	40	R	PU	34
D4.5	Final Infrastructure Deployment Report	4	CMSUC	30	R	PU	41
D5.5	Final Service Support Report	5	CNRS	30	R	PU	41

JRA Deliverables List

Del. no.	Deliverable name	WP no.	Lead beneficiary	*Estimated indicative person-months*	Nature	Dissemination level	Delivery date
D6.1	Interoperability Plan	6	KOLN/CNRS	2	R	PU	3
D7.1	Publishing Tools Plan	7	UU	2	R	PU	3
D8.1	Mining/Integration Tools Plan	8	UCL	2	R	PU	3
D6.2	Interoperability Report 1	6	KOLN/CNRS	20	R	PU	10
D7.2	Publishing Tools Report 1	7	UU	10	R	PU	10
D8.2	Mining/Integration Tools Report 1	8	UCL	10	R	PU	10
D6.3	Interoperability Report 2	6	KOLN/CNRS	40	R	PU	22
D7.3	Publishing Tools Report 2	7	UU	20	R	PU	22
D8.3	Mining/Integration Tools Report 2	8	UCL	20	R	PU	22
D6.4	Interoperability Report 3	6	KOLN/CNRS	20	R	PU	34
D7.4	Publishing Tools Report 3	7	UU	23	R	PU	34
D8.4	Mining/Integration Tools Report 3	8	UCL	25	R	PU	34
D6.5	Final Interoperability Report	6	KOLN/CNRS	14	R	PU	41
D7.5	Final Publishing Tools Report	7	UU	10	R	PU	41
D8.5	Final Mining and Integration Tools Report	8	UCL	15	R	PU	41

For Cycle 1: all deliverables, deliverables to EU and internal deliverables are listed on our WIKI at http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/CycleOne

5. SUMMARY OF MILESTONES AND REVIEWS

5.1 Milestones

List and schedule of milestones

Project Management

Milestone no.	Milestone name	WPs no's.	Lead beneficiary	Delivery date from Annex I [1]	*Comments*
M1.1	Kick-off meeting	WP1	CNRS	Month 3	Full reports available to participants. Summary minutes published on Website
M1.2	Project & Budget Plan Approval	WP1	CNRS	Month 3	
M1.3	VPB meetings	WP1	CNRS	Months 3,10, 22, 34, 42	
M1.4	SAB meetings	WP1	CNRS	Months 9, 21, 33	
M1.5	Revised Project & Budget Plan Approval	WP1	CNRS	Months 10, 22, 34	
M1.6	Approval of Final Project Report & Budget	WP1	CNRS	Month 42	

S/T Coordination of the Network

M2.1	Approval of WP Plan	WP2	CMSUC/CNRS	Month 3	
M2.2	EPT meetings	WP2	CMSUC/CNRS	Months 3, 10, 16, 22, 28, 34, 38, 42	
M2.3	Approval of Revised WP WorkPlan	WP2	CMSUC/CNRS	Months 10, 22, 34	
M2.4	Approval of Final WP Reports	WP2	CMSUC/CNRS	Month 42	

Dissemination and Trainings

M3.1	CTT meetings	WP3	OU/UNIVIE	Months 10, 22, 34, 42	Minutes of Meetings on Internal Website
M3.2	Review of Conferences/Schools	WP3	OU/UNIVIE	Months 10, 22, 34	Agenda and Training material of workshops on Public Website
M3.3	Review of Regional Tutorials	WP3	OU/UNIVIE	Months 10, 22, 34	Agenda and Training material of workshops on Public Website

[1] Month in which the milestone will be achieved. Month 1 marking the start date of the project, and all delivery dates being relative to this start date.

Service Deployment

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

Infrastructure Support

M5.1	Deployment of Monitoring	WP5	CNRS	Months 10, 22, 34, 42	
M5.2	Deployment of Help Desk	WP5	CNRS	Months 10, 22, 34, 42	
M5.3	Deployment of Grid Operation	WP5	CNRS	Months 10, 22, 34, 42	Testing by Users Panels of prototype software
M5.4	Deployment of Preservation and QA	WP5	CNRS	Months 10, 22, 34, 42	Text of Call Available on Public Website

Interoperability

M6.1	Technical Meetings	WP6	UU	Months 5,10, 16, 22, 28, 34, 40, 42	Minutes. Presentations on internal Website
M6.2	Evaluation of standards releases	WP6	UU	Months 10, 22, 34	

Tools to publish A&M Data

M6.1	Technical Meetings	WP7	UU	Months 5,10, 16, 22, 28, 34, 40, 42	Minutes. Presentations on internal Website
M6.2	Evaluation of softwares	WP7	UU	Months 10, 22, 34	

New Mining and Integration Tools

M6.1	Technical Meetings	WP8	UU	Months 5,10, 16, 22, 28, 34, 40, 42	Minutes. Presentations on internal Website
M6.2	Evaluation of softwares	WP8	UU	Months 10, 22, 34	

5.2 Planning of Reviews

Tentative schedule of project reviews

Review no.	Tentative timing, i.e. after month X = end of a reporting period [2]	*planned venue of review*	*Comments , if any*
1	After project month: 12	**13**	Level 1 Service Prototype available from PM 10 on internal Web-Site
2	After project month: 24	**25**	Level 2 Service Prototype available from PM 22 on internal Web-Site
3	After project month: 36	**37**	Level 3 Service Prototype available from PM 34 on internal Web-Site
4	After project month: 42	**43**	Final VAMDC Service Release available from PM 40

6. WP1 ACTIVITIES DESCRIPTION

WP1 is MGT: Project Management

6.1 WP1 Objectives

The VAMDC e-Infrastructure involves 15 partners participants from 6 European Union member states (the CNRS partner involves 6 geographically distributed legal entities), partners in ICPC countries: the Russian Federation, Serbia and Venezuela and external partners in the US. The project will co-ordinate two large Networking programmes; three joint research projects and two supply service activities internally involving some 300 users/providers, and externally providing a transformational set of new services to a wide external audience, during its 42 months programme. The success of the VAMDC e-infrastructure will therefore crucially depend on the effective management and integration of these different elements. The Objective of Work Package 1 is therefore to provide the necessary management structure to implement the VAMDC e-Infrastructure including: handling all administrative matters with respect to EU regulations: assembling and submitting reports, overseeing the audit of the finances, arranging meetings with appropriate staff in Brussels. WP1 will also be responsible for establishing and implementing the higher level strategy of the infrastructure.

WP1 is lead by M.L. Dubernet (CNRS(1)/LPMAA), coordinator of VAMDC.

[2] Month after which the review will take place. Month 1 marking the start date of the project, and all dates being relative to this start date.

6.2 Project Management and monitoring

The Management structure will include a number of Boards, each with well defined remits and responsibilities. The designated Boards are VEB, VPB, SAB as described in section 2.1.

The three main tasks of WP1 are the initial establishment of the management structure and its support communication tools, the regular operation of this structure, and its termination at the end of the project together with the delivery of the final reports.

WP1 Leader	M.L. Dubernet (CNRS/LPMAA)	
Task Number	Leader	Other Partners
1	ML. Dubernet	
2	ML. Dubernet	All others
3	ML. Dubernet	

Task1: Initial establishement of the management structure and tools

Project Months 1 -3 will be entirely devoted to the set-up of the working structure. First, the core of the executive team (Project Coordinator and Project Manager) will be set-up at the coordinating institute (CNRS/LPMAA), and the team will open the project's Central Web Page at CNRS/VOPARIS Data Centre. The Executive Board will establish communication with all consortium members and prepare the project kick-off meeting which will take place at PM 3. The kick-off meeting will include meeting of the VPB, which will choose the SAB and approve the VAMDC project plan.

Task2: Project Management

Following the 'kick off meeting' the project will enter its phase of regular yearly operations, with annual Project Board (10, 22, 34, 42) and SAB (9, 21, 33) meetings. Detailed annual and final reports (PM 12, 24, 36, 42) will be prepared by the Executive Board for presentation to the Board. The report will include review of all the NA, SA and JRAs and include recommendations and comments by the SAB. The report will be reviewed and ratified by the Project Board for transmission to the Commission. Budgetary reports will be assembled by the Project Manager on the Executive Board with particular attention to detailing the spend patterns in the past year and making forecasts for forthcoming year. Should it be necessary to alter spend patterns in forthcoming year the Executive Board will make recommendations to the VPB for their approval. Detailed information on reporting is given below in 6.4.
Detailed annual Project Plans will be prepared by the VEB after gathering all WPs individual project Plans, for presentation to the Board.
Templates for deliverables (reports, plans), internal documents and guidelines will be disseminated.

In other aspects, each WP will monitor the different aspects of its activities. This monitoring is part of the WP internal reports, and will be assessed by the EPT and the VPB.

Task3: Termination of the project

At the end of the project the last task will be the production and delivery to the Commission of the final report and budget.

6.3 Maintenance of the Risk Register and of the Self-Evaluation Matrix

The Risk Register (see section 2.4) has been reviewed and approved by the VPB during the first board meeting. It will be maintained by the VEB.
The VEB will assure the maintenance of the Self-evaluation Matrix for each Work Package (the self-evaluation matrix is updated on line on our WIKI at http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/VamdcPlan). The self-evaluation matrix will be compiled in a PDF document, reviewed and approved by the VPB during board meetings.

6.4 Reporting

Here is a list of documents and reports to be produced during the project and their draft Table of Contents:

WP Plans (D2.1, D3.1, D4.1, D5.1, D6.1, D7.1, D8.1) to be included in the Project Plan (D1.2)

- A description of the Work package activities

Project Plan and Revised Project Plans (D1.2, D1.3, D1.5, D1.7 – WP1)

- A description of the project objectives;
- A description of the Project management;
- A summary of Work Packages, deliverables and milestones;
- A description of the Work packages activities;
- A presentation of the effort distribution;
- An estimated budget breakdown per Work Package.

WP Reports (as indicated in WP activities description) to be included in Budget & Review Report to EU (D1.4, D1.6, D1.8, D1.9)

- A description of the Work package activities

Budget & Review Report to EU (D1.4, D1.6, D1.8, D1.9)
One part of this report is a Periodic activity report, containing:

- A publishable executive summary;
- A description of the project objectives and major achievements during the reporting period;
- An updated version of the Self-evaluation Matrix;
- A description of the Consortium Management;
- A description of the Project Management;

The second part is a Periodic management report, containing:

- A justification of major cost items and resources;
- Financial statement per activity for the contractual reporting period (form C);
- A summary financial report.

The last part of this report is the periodic report on the distribution of the Community's contribution. It shows the distribution of funds made by the coordinator to beneficiaries during the reporting period.

7. WP2 ACTIVITIES DESCRIPTION

WP2 is NA1: Science/Technical Coordination of the network

7.1 WP2 Objectives

NA1 provides the scientific and technical work necessary for the operation of the VAMDC e-infrastructure developing its structures and integrating with other data services and placing the VAMDC in a more global context. NA1 will also provide effort for VAMDC to participate and interact with external infrastructure and standards groups such as EGEE, Euro-VO and the IVOA.

The organisation of WP2/NA1, and the technical coordination of the network, is overseen by the VAMDC Executive Project Team (EPT)

The EPT includes WPs leaders (WP2 to WP8). The EPT will have monthly teleconference meetings as well as bi-annual face-to-face meetings. It will collect reports from the SAs and JRAs and prepare the annual technical reports for the VPB. The EPT will be chaired by the VAMDC Deputy (Technical) Coordinator who is a member of the VAMDC Project Board and will advise the VPB on the technical validity and relevance of the project strategic plans.

WP2 leader is CMSUC (2), with co-leadership by CNRS(1)

7.2 WP2 Milestones and Deliverables

Milestones

M2.1	Approval of WP Plan	WP2	CMSUC/CNRS	Month 3	
M2.2	EPT meetings	WP2	CMSUC/CNRS	Months 3, 10, 16, 22, 28, 34, 38, 42	
M2.3	Approval of Revised WP WorkPlan	WP2	CMSUC/CNRS	Months 10, 22, 34	
M2.4	Approval of Final WP Reports	WP2	CMSUC/CNRS	Month 42	

Deliverables

D2.1 Science / Technical (S/T) Plan (PM 3)

Annual reports will provide publicly available summaries of the activity of the EPT for each project year.

D2.2 S/T Report to be included in report to EU– Year 1 (PM 10)

D2.3 S/T Report to be included in report to EU– Year 2 (PM 22)
D2.4 S/T Report to be included in report to EU – Year 3 (PM 34)
D2.5 Final S/T Report to be included in final report to the EU (PM41)
Annual S/T Plan revisions included in Revised Annual VAMDC Project Plans – Year 1,2,3

Internal deliverables for year 1 activities are listed below.

7.3 WP2 Tasks Description

WP2 Leader	N. Walton (CMSUC(2)), M.L. Dubernet (CNRS/LPMAA)	
Task Number	Leader	Other Partners
1	N. Walton (CMSUC)	All others
2	N. Walton (CMSUC)	All others
3	T. Ryabchikova (INASAN)	All others
4	E. Roueff (CNRS/LUTH)	All others
5	E. Roueff (CNRS/LUTH)	All others

Task 1: Internal Technical Activities (lead by CMSUC(2), all partners)
Task 1 deals with cross disciplinary technical coordination, identification and evaluation of proposed generic tools, preparation of plans for testing and benchmarking activities. This task also includes the organisation of the EPT meetings.

Task 2: Connection to External Technical Project (lead by CMSUC(2), partners 1,3,4,14)
Task 2 deals with coordination with IVOA (International Virtual Observatory Alliance), Euro-VO, the IDIS Data service of the Europlanet EU Research Infrastructure, EGEE (European Grid E-science Environment). The EPT will host annual small focussed meetings/workshops where relevant people from the external projects will be invited to present the status of their achievements. The EPT will assess the degree of interoperability with those projects, which will in turn influence the output of task 1.

Task 3: Collect the users and producers specifications (lead by INASAN(15), all partners)
The EPT will gather users/producers requirements by a number of techniques such as questionaires, small face-to-face meetings and so forth.

Task 4: Policies concerning Standards (lead by CNRS(1), all partners)
Task 4 will define, review and update the way standards will be adopted and to that effect it will interact with organisations promoting standards, e.g. external projects cited in task 2, NIST project for defining units in XML schema. Other organisations will be identified during the project if they happen to be relevant to VAMDC.

Task 5: Policies concerning publication in VAMDC (lead by CNRS(1), all partners)
Other missions of the EPT are to define, update and maintain the policies concerning the publication of resources in VAMDC.

7.4 WP2 Tasks Description for Period 1

Full task activities are detailed at the VAMDC wiki on the WP2/NA1 pages – see http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/WP2

Task 1: Internal Technical Management

- The EPT meetings occur once every two months, with the kickoff EPT-0 meeting 7 Oct 2009 (see http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/EptTeleOct2009). All EPT meetings are fully minuted at http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/Na1Ept
- NA1 will organise representation at partner VAMDC related meetings
  - High-Russ 2009 Conference, Lake Baikal, July 2009
  - Conferencia Latinoamericana de Computación de Alto Rendimiento: CLCAR-2009: Merida, Venezuela, Sep 2009
- In coordination with SA1, a census of all VAMDC resources will be undertaken (M4)
- A VAMDC standard tool set will be determined and introduced (M6)
- The quality assurance systems for VAMDC will be defined (M9) and introduced at the second project meeting.

Task 2: External Coordination.

Project representatives will coordinate with relevant external partners, directly and through EC organised events:

- 7th Concertation meeting on e-Infrastructure (FP7 funded test beds) in Brussels (Belgium) (12-13 Oct 2009) – see http://www.beliefproject.org/events/7th-e-infrastructure-concertation-meeting
- Attendance at the IVOA InterOp meetings
  - Autumn 2009 – Nov 2009 @ ESO, Garching, Germany
  - Spring 2010 – May 2010 @ CADC, Victoria, Canada
- Attendance at Euro-VO Technology Forum meetings
  - see http://cds.u-strasbg.fr/twikiAIDA/bin/view/EuroVOAIDA/AIDASchedule
- Attendance at relevant EuroPlanet IDIS technical meetings.
  - See http://www.europlanet-ri.eu/idis
- Attendance at relevant EGEE and EGI technical meetings
- VAMDC external technical workshops – two will be organised in the first year
  - Data Access (M6)
  - Applications and run time environments (M9)

Task 3: User / Producer specifications

- The main activity will be in organising a census of user specifications
  - Initial requirements gathering at Kick-Off meeting – Paris Oct 26-27 2009
  - Census of requirements (M6)
  - Report of requirements for inclusion in year one technical plan (M9)

Task 4: Standards Policies

- Development of standards policy
  - Initial discussion at Annual meeting April 2010
  - Release of preliminary standards policy to VAMDC website (M11)

Task 5: Publications Policies

- Development of publication policy
  - Initial discussion at Annual meeting April 2010
  - Release of preliminary publication policy to VAMDC website (M11)

8. WP3 ACTIVITIES DESCRIPTION

WP3 is NA2: Dissemination and Training

8.1 WP3 Objectives

Our objective is to attract new participants to the e-infrastructure, i.e. producers and users of data.
The key objective of the training and dissemination activity is to ensure that principle stakeholders are engaged in the development and implementation of the VAMDC E-infrastructure. This Work package will therefore provide for:
a) Dissemination of VAMDC services at national, EU and non-EU levels
b) Training of producers & users at master, PhD and professional levels (both academic and non-academic users)
Specifically this work package provides for:
1) An annual meeting, which showcases the work of the e-infrastructure, supports networking and scientific communication, and becomes the conference of choice for users and providers of atomic and molecular data
2) Organize topic based scientific workshops, twice a year, to bring together proposers, users and providers of A&M data to discuss data needs and how VAMDC can meet those needs.
3) Arrange teaching tutorials (on-line and face to face) on the VAMDC e-infrastructure

8.2 WP3 Milestones and Deliverables

Milestones

M3.1	CTT meetings	WP3	OU/UNIVIE	Months 10, 22, 34, 42	Minutes of Meetings on Internal Website
M3.2	Review of Conferences/Schools	WP3	OU/UNIVIE	Months 10, 22, 34	Agenda and Training material of workshops on Public Website
M3.3	Review of Regional Tutorials	WP3	OU/UNIVIE	Months 10, 22, 34	Agenda and Training material of workshops on Public Website

Deliverables

D3.1 Dissemination and Training (D&T) Plan (PM 3)
D3.2 Annual D&T Report to be included in report to EU – Year 1 (PM 10)

Annual reports will provide publicly available summaries of the activity of the WP for each project year. Report will include a list of meetings/conferences attended to disseminate VAMDC to other communities. Annual reports will be for examined by the VAMDC Project Board.
D3.3 VAMDC Level 1 Service Prototype (PM10)
D3.4 VAMDC Annual Project Meeting 1 at OU (4) (PM12)
An annual meeting will be organized at the end of each year of the project
D3.5 Annual D&T Report to be included in report to EU – Year 2 (PM 22)
D3.6 VAMDC Level 2 Service Prototype (PM22)
D3.7 VAMDC Annual Project Meeting 2 at CMSUC (2) (PM24)
D3.8 Annual D&T Report to be included in report to EU – Year 3 (PM 34)
D3.9 VAMDC Level 3 Service prototype (PM34)
D3.10 VAMDC Annual Project Meeting 3 at UNIVIE (5) (PM36)
D3.11 VAMDC Service Release (PM40)
D3.12 VAMDC Final Annual Project Meeting at CNRS (1) (PM42)
D3.13 Final Report of Dissemination and Training to be included in final report to the EU (PM42)
The final report will include a reflexive analysis of the effectiveness of the WP, and proposals for future activities beyond the lifetime of the project. This deliverable will be organized under Task 1.

Annual D&T Plan revisions included in Revised Annual VAMDC Project Plans – Year 1,2,3

8.3 WP3 Tasks Description

WP3 Leader	N. Mason (OU)	
Task Number	Leader	Other Partners
1 Coordination	N J Mason (OU)	F. Kupka (UNIVIE)
2 Annual meetings	N J Mason (OU)	All partners involved in WP3
3 Scientific Workshops	N J Mason (OU)	All partners involved in WP3
4 Training Tutorials	N Walton (CMSUC)	UCL; CPTM, INASAN, IAO
5 VAMDC Service	N Walton (CMSUC)	UU - CNRS

Description of work

This activity provides the conduit for communicating both the aims and results of the VAMDC e-infrastructure. Dissemination activities are aimed at VAMDC's users, the wider European science community, European industrial stakeholders and policy makers. It is intended to provide an attractive platform to exchange and present results, develop new ideas and to network with other data providers and e-infrastructures. This will be accomplished by organizing a high profile annual meeting, being represented at other appropriate conferences and hosting a series of targeted topical workshops and teaching tutorials.

NA2 therefore consists of four tasks:
1) Coordination
2) Organizing an annual meeting and arranging representation at other relevant meetings
2) Organizing themed scientific workshops

3) Organizing training tutorials

Task 1: Coordination (Chair OU(4), Deputy Chair UW_A(5))

Dissemination activities will be a pre-requisite for all VAMDC's activities. Therefore each NA, SA and JRA will nominate a member to prepare the necessary material for disseminating the aims, objectives and results of these activities. Dissemination across the project will be coordinated by the **Communication and Training Committee (CTC).** The role of the communication and training committee is to propose a list of dissemination and training actions, to organize the general events linked to this project and to compile records of actions. It will be composed of NA2 partners and chaired by the WP3 leader (OU). The CTC will organise the communication and training section of the VAMDC web-site. This section will hold all records of dissemination and training actions and the CTC will be responsible for updating this section with announcements, news, proceedings, and presentations.

Task 2: Organisation of annual international conference and VAMDC's representation at other relevant meetings

Annual meeting The CTC will organise an annual international conference focused on the VAMDC e-infrastructure, its resources and services. The programme committee will be chaired by OU with UNIVIE as deputy. It will be aimed at users, producers and developers. It will include both academic and non-academic users. This major event will be held each year in a different part of the EU and proceedings will be published (both on line and subject to discussions with scientific publishers in hardcopy – note the UK Institute of Journal of Physics Conference Series have expressed interest in publishing such proceedings).

It is VAMDC's ambition that this meeting become a conference of choice for A&M database providers and for A&M data users (We wish at least one meeting to be combined with the international ICAMDATA conference).The conference will therefore aim to attract a wide audience including many of the key stakeholders we wish to engage with (industrialists, politicians, media). The Conference will also be the location of many of the VAMDC e-infrastructure's necessary management meetings.

Dissemination via EU national and international existing conferences

Yearly the CTC will establish a list of national and international conferences where oral presentations and demonstrations on VAMDC will be valuable. These national and international conferences will usually be conferences of producers and users. AOB will be responsible for collating the information and arranging with other partners VAMDC presence at such meetings. The CTC will accordingly prepare suitable display material (in electronic format and hard copy) for display at such meetings which can be *used by any of the VAMDC partners.*

Organisation of "regional" tutorials

Since the VAMDC e-infrastructure is planned as an international activity and includes international partners the CTC will also prepare a list of tutorials that will be held in non-EU countries in order to spread the knowledge and practice of the VAMDC infrastructure. These tutorials will be organised by our non-EU partners (CPTM, INASAN, IAO, AOB) and will be aimed at people from those "regions".

Task 3: Scientific workshops

Central to the aims of the VAMDC is the formation of an infrastructure that responds to the needs of its user communities since the major impact of the e-infrastructure will be its adopting by scientific and technology communities. Therefore in order to ascertain the requirements of current and potential VAMDC communities and in order to inform the project we will host a series of themed workshops with such communities. These meetings may be stand alone or more usefully as part of the user community's own conference/meetings programme (through arranged VAMDC sessions). It is anticipated that two such meetings would be per year. Administration of these meetings will be arranged by the CTC.

Proposed topics follow those identified in Section 3 (Impact) and include; The astronomical and planetary science Community (with sessions held at the Euro planet RI meeting, SF2A, IAU meetings); The atmospheric science community (in collaboration with one of the HITRAN database meetings); The technology plasma community (at its European meeting ESCAMPIG); The fusion community (as part of the IAEA meetings for ITER itself part of the EURATOM programmed); The Lighting industry (hosted by Philips ltd) and the radiation sciences community (possibly in collaboration of GEANT meeting and the EU RADAM conference series). Each of the following partners will organize (and when necessary host) one or more such workshops; OU (plasma and radiation sciences); UCL and IAO (atmospheric science and Hitran); CMSUC, AOB, CNRS (astronomy and planetary science); UNIVIE and OU (fusion (with IAEA) and lighting).

Task 4: Training Tutorials

CMSUC and UCL will prepare material for the partners to use in training workshops both in their own countries and internationally. These tutorials will be focused in developing a user's competence to use the e-infrastructure and to interface it into their own operating systems; Short training sessions will be integrated into the Annual meeting. All partners will be required to nominate one member who will be able to 'train' and/or provide support for their national users. Our non EU partners (CPTM, INASAN, IAO) will also prepare a self-studying e-tutorial for VAMDC users who can not attend such tutorials. We (OU,UCL) will also prepare an e-tool for general public/more general stakeholders such that they can take a virtual guided tour of VAMDC including its current status: statistics, content, geography of clients and producers etc.

Task 5: VAMDC Service & Service Prototype Release

CMSUC, UU and CNRS will lead the coordinated release of the annual VAMDC prototype service. This will lead to the final release of the VAMDC service infrastructure. The annual prototypes will be reviewed at the yearly project meetings and available for assessment alongside the VAMDC annual reports.

The prototype services will contain the following functionality:

Level 1: Preliminary VAMDC service with simple data access to the core VAMDC data resources
Level 2: Enhanced interoperable data access to VAMDC data resources, all resources accessible
Level 3: Interoperable VAMDC data access with VAMDC tools available (client side or server side accessible via through workflow enactment engines)
VAMDC Service: Final full service, including access to resources from the wider community (through the SA1 / Task 6 community call).

8.4 WP3 Tasks Description for Period 1

Internal Deliverables:

Task 1; Dissemination activities are a pre-requisite for all VAMDC's activities. Therefore every activity NA, SA and JRA and Partner will provide nominated members for their activities and organisation with which the **Communication and Training Committee (CTC)** can interact. The CTC itself will be composed of NA2 partners and chaired by N J Mason (OU).
Establish membership of the CTC by April 2010
Meeting of CTC at first annual meeting in April 2010 at OU in UK
The CTC will ensure each partner has an appropriate VAMDC website and design the VAMDC dissemination webpages

Task 2: Organisation of annual international conference and VAMDC's representation at other relevant meetings

To organise the first Annual meeting of the VAMDC infrastructure.
To be held in the UK in April 2010 at or close to Open University. Meeting to include meetings of necessary Boards and CTC. Conference to include a training tutorial and scientific workshop.

To determine meetings and conferences at which VAMDC to be represented and CTC to prepare material for distribution at these meetings. To arrange session at European Planetary Science Congress and discussion with IDIS database providers

Regional Tutorials to be held in non-EU partners venue and timings to be arranged for project.

Task 3: Organization of Scientific workshops

Programme of scientific workshops to be determined, with dates and venues
Workshops for 2010 may include joint meetings with RADAM (Madrid June 30 –July 2) on radiation damage and ESCAMPIG (Novi Sad Serbia July 13-17).

Task 4: Training Tutorials

CMSUC and UCLto prepare material for the partners to use in training workshops both in their own countries and internationally. These tutorials will be focused in developing a user's competence to use the e-infrastructure and to interface it into their own operating systems;

All partners will be required to nominate one member who will be able to 'train' and/or provide support for their national users.

Non partners (CPTM, INASAN, IAO) will also prepare a self-studying e-tutorial for VAMDC users who can not attend such tutorials.

OU, UCL will also prepare an e-tool for general public/more general stakeholders such that they can take a virtual guided tour of VAMDC including its current status: statistics, content, geography of clients and producers etc.

Task 5: VAMDC Service & Service Prototype Release

To develop methodology for coordinated release of the annual VAMDC prototype service.

First presentation at first annual meeting in April 2010. The prototype services will contain the following functionality:

Level 1: Preliminary VAMDC service with simple data access to the core VAMDC data resources

9. WP4 ACTIVITIES DESCRIPTION

WP4 is SA 1: Infrastructure Deployment

9.1 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)

9.2 WP4 Milestones and Deliverables

Milestones

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

9.3 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	TBD (UCL) – not cycle 1	TBD
5	TBD (CNRS) – not cycle 1	TBD
6	TBD (CNRS) – not cycle 1	TBD

Description of work (possibly broken down into tasks)

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 (5), (6))
Where a VAMDC node has a useful numerical code for AM analysis or modeling, 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.

9.4 WP4 Tasks Description for Period 1

Task 1: Standard access to AM data

Task 1.1 TAP access to A-M data

Using existing software from the Virtual-Observatory movement, implement Table Access Protocol (TAP) services for sample nodes with data in relational databases.

TAP is the IVOA standard for remote access to relational databases. It is a low-level protocol, applicable to A-M physics as well as astronomy, suitable for prototyping VAMDC applications and workflows. Because complete, reusable, TAP software is available to us at no cost, TAP is a cheap way to make data available in year 1 of VAMDC before the VAMDC-specific web-services are defined.

Various databases will be selected for this trial according to schedule: CHIANTI, XSTAR, VALD, BASECOL, CDMS.

Task 1.2 Ingest data into databases

Ensure that all data-publishing nodes in VAMDC have their data copied into database systems suitable for supporting the VAMDC-standard web-services to be defined by WP6 and WP7.

Some VAMDC partners already have their data-sets stored in relational databases; others keep their data in flat files. The web services foreseen in the early planning require all data to be loaded into some kind of database. The exact kind of database depends on the design of the services.

Task 1.3 Install early prototypes of VAMDC-standard data-access services

Acquire an implementation of the VAMDC-standard data-access service, as defined by WP6 and implemented by WP7. Install this on all VAMDC node that have achieved a suitable database (as per task 1.2). Register the data-access service in the VAMDC registry.

These VAMDC-standard services will probably be based on the XSAMS data-model, possibly using the XQuery query-language. They operate at a higher semantic-level than the TAP services.

This task presumes that WP6 and WP7 produce a design and implementation suitable for wide deployment. It is possible that the new software does not become sufficiently mature for full deployment by the end of period 1. To conserve resources, two sites should be chosen for test deployment and evaluation before the software is deployed on all sites.

Task 2: Standard access to numerical codes

Task 2.1: Make a census in order to inventory numerical codes likely to be turned into public services

Task 2.2: Propose solutions to establish services in order to launch codes in VAMDC environment – Test solution on one or two codes

Task 3: Implementing registries

Task 3.1 Choose a host for the VAMDC registry

Select a VAMDC partner to run the registry.

In period 1, we need only one registry on a single site. Towards the end of the VAMDC project we may set up a mirror of this registry on a separate site.

Task 3.2 Install registry software
Install the AstroGrid registry-service component at the chosen registry site. Establish registry access for all VAMDC partners who need to register resources.

The registry software for this task is a web service available ready-to-run from AstroGrid. The task does not include populating the registry with information; when the task is complete, the registry will be available to publishers but will not contain all the metadata needed by end users.

Task 3.3 Register existing resources
Register the existing, web-browser interfaces to data sets.

Task 4: Augmenting VODesktop
Task 4.1 Distribute TAP-capable copy of VODesktop
Ensure that all VAMDC staff have access to a version of VODesktop that works with the early-access TAP services. Make this software available for download from the VAMDC site.

By the time that VAMDC needs it, the default version of VODesktop should be suitable.

Task 4.2 Extend VODesktop to work with VAMDC-standard data services
Add code to VODesktop such that it can query the new prototypes of the VAMDC data-services deployed in task 1.3.

This task is only possible once WP6 designs the service protocol. If that design is not stable during period 1, it is not worth altering VODesktop; instead, we should produce simpler, disposable clients to test the services.

Internal deliverables

- TAP services for selected sites – month 7
- VAMDC-standard data-access services – month 9
- Registry service, ready for publishing, not fully populated – month 6
- Registration of web-browser (pre-VAMDC) interfaces – month 7
- VODesktop version for TAP services – month 4

10. WP5 ACTIVITIES DESCRIPTION

WP5 is SA 2: Support to the Infrastructure

10.1 WP5 Objectives

SA2 provides support for the delivery of the VAMDC e-infrastructure to users and producers (SA1) . SA2 will be responsible for the maintenance and monitoring of the core infrastructure;

Implementing Grid technology within the VAMDC: providing direct support to the users of the scientific data infrastructure as they enter the VAMDC portal and for the preservation and storage of digital data.

WP5 Leader is CNRS(1)

10.2 WP5 Milestones and Deliverables

Milestones

M5.1	Deployment of Monitoring	WP5	CNRS	Months 10, 22, 34, 42	
M5.2	Deployment of Help Desk	WP5	CNRS	Months 10, 22, 34, 42	
M5.3	Deployment of Grid Operation	WP5	CNRS	Months 10, 22, 34, 42	Testing by Users Panels of prototype software
M5.4	Deployment of Preservation and QA	WP5	CNRS	Months 10, 22, 34, 42	Text of Call Available on Public Website

Deliverables

D5.1 Service Support Plan (PM 3)
D5.2 Infrastructure Support Report to be included in report to the EU– Year 1 (PM 10)
D5.3 Infrastructure Support Report to be included in report to the EU – Year 2 (PM 22)
D5.4 Infrastructure Support Report to be included in report to the EU – Year 3 (PM 34)
D5.5 Final Report of Service Support to be included in final report to the commission (PM41)
Annual Service Support Plan revisions included in Revised Annual VAMDC Project Plans – Year 1,2,3

10.3 WP5 Tasks Description

WP5 Leader	P. Le Sidaner / K. Benson CNRS:UMS / UCL :MSSL	
Task Number	Leader	Other Partners
1	A.Shih (CNRS:UMS)	All
2	L.A. Molina (CNRS:LUTH, LPMAA)	All
3	Not yet decided as it starts on M12	
4	P. Le Sidaner (CNRS: UMS)	All
5	Not yet decided as it starts on M12	

Description of work (possibly broken down into tasks)

Task1: Maintenance and monitoring of the core infrastructure (CNRS(1), all SA2 partners)

The core infrastructure will include partners who maintain existing databases and services. All the actors will be in charge of providing access to the databases/services deployed in SA1. The services include accessing the databases via different protocols, access to dictionaries and publishing registries. Task1 involves setting up the quality assurance of the infrastructure activities, service heartbeats and development and use of unit test packages. The monitoring

activities will be implemented at VO-Paris Data Centre using the NAGIOS software. We will need to develop plugins specific to the various protocols which will need validation. Monitoring Software implemented at VOPARIS Data Centre will be distributed to regional centres.

Task 2: Grid Operations (CNRS(1))

The infrastructure includes the possibility to use the GRID technology in order to run numerical codes that produce AM data or that use AM data on hardware provided outside VAMDC. This is separate from and complementary to the execution of codes on hardware provided at VAMDC nodes (the latter facility is part of SA1). Task 2 will make selected codes useable on the grid. The work involves:

- making the codes executable on grid nodes, either by making the codes themselves portable or by packaging them in virtual machines;

- providing grid portals where the codes can be invoked and from which the results can be retrieved;

- negotiating access for VAMDC users with grid providers, especially with EGEE

Task 3: Support to "users" of the infrastructure (UCL(3) with partners (2), (12), (15))

"Users" of the infrastructure, meaning all people interacting with the infrastructure, will need to have access to information concerning the composition of the infrastructure, the services which are available, the procedures about how to enter the infrastructure, the procedures about how to implement the standards, how to use or adapt the various tools. The support to the "users" will be operated in Task 3 through the provision of on-line support materials, a help desk and a service providers/users forum where people could share best operation practice. We intend to produce a self-studying e-tutorial that can be incorporated in university courses on molecular and atomic physics, astronomy, energy systems, environment (etc). Also we intend to operate an e-tool for general public to take a virtual guided tour of VAMDC: statistics, content, geography of clients and producers, databases locations. Dissemination and Tutorials organized in WP3 will show and teach how to implement and use the infrastructure, will advertise all those tools. Note that the actual generation of the training materials and support events will be organised by WP3 (NA2).

Task 4: Preservation of digital data and resources (CNRS(1))

The Preservation of digital data and resources is one of the key aspect of sustainability. It is the purpose of SA3 to set up a system of preservation through archiving and mirroring. Some nodes will act as repositories: the nodes already supporting such preservation (nodes linked to VALD, CHIANTI, etc..), VOPARIS Data Centre which will act for most of CNRS resources and could be extended to other partners. The first proposed technology will be to create a virtual machine for a certain number of projects who will implement their resources and we will implement synchronisation. This first step of a mirroring site is the simplest approach and will be implemented during the whole project. During Phase 1 we will work at the EPT level in order to follow preservation activities in other areas. We will adjust our preservation policy accordingly in Phase 2.

Task 5: Quality Assurance of data and resources (CMSUC(2), with partners 3, 11, 12, 15)

Another crucial point is the reliability of the data transferred via the various protocols. The database providers are responsible for the entries in their own database. The usual and slow way of accessing data via classical web interface or via ftp obliges the user to understand the structure of the database, to read instructions in order to get the meaning, definition of columns and lines. An interoperable e-infrastructure will remove some of this verification process of the user. Therefore it is indispensable to check that all resources (core and new

ones) use the protocols, standards in the best and reliable way. In Task 5 small groups of VAMDC people understanding the protocols/standards and the physics of the retrieved data will test the output of databases in order to check the good use of protocols, whenever there is a new release handling new cases.

10.4 WP5 Tasks Description for Period 1

Task 1: Maintenance and monitoring of the core infrastructure

- 1.1 Install of Nagios (M6)
- 1.2 The list of machines and services to monitor as well as contacts will be defined by the first 9 months and will be updated over time. Using existing plug-ins or defining new.
- 1.3 New plug-ins will depend on the protocol defined inside VAMDC
- 1.4 Installation and maintenance of the monitoring process for machines and services

Task 2: Grid Operations

- 2.1 Making an inventory of codes where grid launch should be useful : this task has to be started by the first 7 months (codes producing A&M data or application codes using A&M data) - Provide List of codes
- 2.2 Gridify codes if necessary and test codes in EGEE grid - Use 2 codes and Record Pbs, edit documentation - Starting Month 7
- 2.3 Find the most useful portal for launching and monitoring these codes on the Grid– Provide Documentation- Starting Months 7

Task 3: Support to "users" of the infrastructure – Starts only on Month 12 (Cycle 2)

Task 4: Preservation of digital data and resources

- 4.1 After first inventory of services, some more point will be defined by contacting contact persons for services at each node res:
  - What technologies to be used (OS, BDD, language required, total volume ...)
  - Who will be the technical contact to give access to for replication of service
  - Who will be the scientific contact who will validate mirror
- 4.2 This jobs will be start just after inventory (and only for few sites):
  - Virtual machine installation (M11)
  - Negotiation on each service (M11)
  - Installation of services and replication process for chosen sites (M11)

Task 5: Quality Assurance of data and resources - Starts only on Month 12 (Cycle 2)

11. WP6 ACTIVITIES DESCRIPTION

WP6 is JRA1: Interoperability

11.1 WP6 Objectives

Define all standards necessary to build an interoperable infrastructure

WP6 Leader is KOLN with co-leader CNRS

11.2 WP6 Milestones and Deliverables

Milestones

M6.1	Technical Meetings	WP6	UU	Months 5,10, 16, 22, 28, 34, 40, 42	Minutes. Presentations on internal Website
M6.2	Evaluation of standards releases	WP6	UU	Months 10, 22, 34	

Deliverables

D6.1 Interoperability Plan (PM 3)
D6.2 Interoperability Report to be included in report to the EU – Year 1 (PM 10)
D6.3 Interoperability Report to be included in report to the EU – Year 2 (PM 22)
D6.4 Interoperability Report to be included in report to the EU – Year 3 (PM 34)
D6.5 Final Report of Interoperability to be included in final report to the commission (PM41)
Annual Interoperability Plan revisions included in Revised Annual VAMDC Project Plans – Year 1,2,3

11.3 WP6 Tasks Description

WP6 Leader (co)	S. Schlemmer (KOLN)/ M.L. Dubernet (CNRS: LPMAA/LUTH)	
Task Number	Leader	Other Partners
1	M.L. Dubernet/J. Bureau (CNRS:LPMAA/LUTH)	All partners
2	T. Millar (QUB)	All partners
3	N. Piskunov (UU)	CNRS:LPMAA/LUTH
4	M. Doronin (CNRS:LPMAA)	UU
5	S. Schlemmer (KOLN)	All partners

Description of work (possibly broken down into tasks)

Task 1: Data Models and XML Schema (lead by CNRS(1), all JRA1 partners)
The current data models and XML schema are a description of atomic and molecular linelists for use in an astrophysical context and a description of atomic and molecular elementary processes. The documents have been designed by a small number of people, those documents are still in draft mode, do not cover all application fields and have not been discussed extensively among users and producers. These preliminary versions will be completed and extended in order to cover a wider range of species, a wider range of processes and will include the effect of the environment. For now we identify the following extensions:

- inclusion of solid, surface spectroscopy for interstellar medium and planetology
- inclusion of larger molecules such as PAH
- description of atomic and molecular line shapes arising from different sources

In connection to the user & producer board of NA2, more extensions will be considered if necessary. Through the Standards and Processes Committee all standards will be connected to International efforts of standardisation.

Task 2: Dictionaries (lead by QUB(9), all JRA1 partners)

In order to uniquely identify resources we will need to define and build dictionaries both general and specific to applications. At present we identify the following dictionaries:
- single identification of databases and services
- list of conventions (link to IUAPAC and other convention bodies)
- list of names of species (in relation with other fields such as chemistry)
- list of processes and coding of processes
- list of quantum numbers

Other lists will be identified during the course of the project in relation with activities in WP2 (NA2)

Task 3: Access Protocols and Query/Retrieval Languages (lead by UU(6), all JRA1 partners)

We will define protocols retrieving different types of resources: numerical data, libraries, documentation, references. Those protocols will cover asynchronous queries and the retrieval of huge sets of data. In a second step we will design a general query language allowing to access and retrieve any atomic and molecular data.

Task 4: Registries (lead by CNRS(1) with partner 6)

Registries provide a mechanism with which applications can discover and select resources--e.g. data and services--that are relevant for a particular scientific problem. We will start from the registries defined in the IVOA and see how to adapt and/or extend the documents to our own purpose. In particular we wish to implement ways of finding resources at various levels of granularity.

Task 5: Other Documents (lead by KOLN(7), all JRA1 partners)

Other basic definitions/standardisations might be necessary in order to find/identify resources and documents produced by the IVOA will be assessed in order to keep/adapt to our own needs.

11.4 WP6 Tasks Description for Period 1

Full task activities are detailed at the VAMDC wiki on the WP6/JRA1 pages – see http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/WP6

Task 1: Data Models and XML schema Documents

- 1.1 – Investigation of XSAMS – Leader CNRS/LPMAA with all participants -
  - Presentation of XSAMS at Kick-Off (M4)
  - Investigation of Molecular Parts by Partners (M4-M9)
  - Produce document where modifications to XSAMS is proposed by M9 –
- 1.2 – Schema for Solid Spectroscopy - Leader CNRS/LPG with internal and external partners (EuroPlanet RI FP7 project)
  - Organisation of Solid Spectroscopy Workshop to discuss Schema (M7)
  - Draft documents M9; M11
- 1.3 – Schema for PAH – Leader INAF + CNRS/CESR
  - Draft documents M9; M11

- 1.4 – Schema for Line Shapes related to pressure broadening – Leader UCL with participants CNRS/GSMA, ICB, IAO, CFA
    - Draft documents M9; M11
- 1.5 – Schema for Atomic Line Shapes – Leader AOB + CNRS/LERMA
    - Draft documents M11

Task 2: Dictionaries Documents

Drafts of lists will be provided in M9 and updated in M11

- 2.1 List of Species Names: make decision about standardized names
- 2.2 List of Processes: complete the list of processes given in XSAMS
- 2.3 List of Conventions
- 2.4 List of Quantum Numbers: complete the list of processes given in XSAMS

Task 3: Access Protocols and Query/Retrieval Language Documents

- 3.1 – Understand existing protocols – Leader CNRS/LPMAA with UU
    - Draft Documents M9, M11
- 3.2 – List of Requirements Application Fields in connection with User/Producer requirements of WP2 – Leader UU with CNRS/LPMAA
    - Draft Documents M11
- 3.3 – Make Proposition – Leader UU with CNRS/LPMAA
    - Draft Documents M11

Task 4: Registries Documents

- 4.1 – Understand existing protocols – Leader CNRS/LPMAA with UU
    - Draft Documents M9, M11
- 4.2 – List of Requirements Application Fields in connection with User/Producer requirements of WP2 – Leader UU with CNRS/LPMAA
    - Draft Documents M11
- 4.3 – Make Proposition – Leader CNRS/LPMAA with UU
    - Draft Documents M11

The documents will be available within the consortium during the whole project on the private part of our web-site. We plan a public release of draft/final versions on our public web-site at Months 12

12. WP7 ACTIVITIES DESCRIPTION

WP7 is JRA2: Publishing Tools

12.1 WP7 Objectives

Provide generic tools partly using the standards developed in JRA1 in order to help producers of A&M data to publish their sets into the VAMDC infrastructure.

WP7 Leader is UU(6)

12.2 WP7 Milestones and Deliverables

Milestones

M7.1	Technical Meetings	WP7	UU	Months 5,10, 16, 22, 28, 34, 40, 42	Minutes. Presentations on internal Website
M7.2	Evaluation of softwares	WP7	UU	Months 10, 22, 34	

Deliverables

D7.1 Publishing Tools Plan (PM 3)
D7.2 Publishing Tools Report to be included in report to the EU – Year 1 (PM 10)
D7.3 Publishing Tools Report to be included in report to the EU – Year 2 (PM 22)
D7.4 Publishing Tools Report to be included in report to the EU – Year 3 (PM 34)
D7.5 Final Report of Publishing Tools to be included in final report to the commission (PM41)

Annual Publishing Tools Plan revisions included in Revised Annual VAMDC Project Plans – Year 1,2,3

12.3 WP7 Tasks Description

WP7 Leader (co)		
Task Number	Leader	Other Partners
1	M.-L. Dubernet/M. Doronin (CNRS)	All others
2	M.-L. Dubernet/M. Doronin (CNRS)	All others
3	N. Piskunov (UU)	All others
4	P. Loboda (RFNC-VNIIT)	All others
5	A. Fazlief (IAO)	All others

Description of work (possibly broken down into tasks)

This WP will develop software that will be deployed within the VAMDC infrastructure. Some of these software will be associated to the standards developed in JRA1. The general software made available to the community will be accessible via the VAMDC technical web-site. Two alternative variants are being developed. The first one implies the design of software for the process of existing information resources transformation into standardized (tasks 2-4) forms set in JRA1. The second variant implies the design of a typical information system accessible via the Internet (task 5) and having an integrated tool developed in tasks 1-3. In this variant automatic generation of semantic metadata for uploaded information resources is realized, taking into account the restrictions imposed by formal models of molecules and atoms. All software will be documented.

During the course of the project additional software might be. The EPT will decide upon the new developments to be carried out by the partners involved in WP8.

The following software are aimed at enhancing scientific research through allowing easy and secure publication of A&M resources within the VAMDC infrastructure:

Task 1: Create/adapt tools to go from an DM/XML schema to a full database deployment with generation of automatic administrative interface. ***(lead by CNRS(1) with (6))***
Task 2: Create/adapt tools to build registries from the content of databases ***(lead by CNRS(1) with (6))***
Task 3*:* Create/adapt interfaces to easily update dictionaries ***(lead by UU(6) with (1))***
Task 4: Develop software libraries using various languages allowing to easily generate output of already existing resources in standardized format ***(lead by RFNC-VNIIT(12) with(1), (6), (8))***
Task 5: Create tools to upload, modify, retrieve, compare, visualize and publish information in molecular spectroscopy ***(lead by IAO(13))***

12.4 WP7 Tasks Description for Period 1

The WP7 Work Plan includes final products of two types: formulation of a number of procedures and development/adoption of a number of software tools. Several tasks in the WP7 are closely related to other work packages and require close and intensive collaboration.

The procedures to be formulated for the Publishing Tools WP7 are:

- *Preparation rules for the original data.* We intend to offer reasonable flexibility for the format of data sets to be imported to a VAMDC database but the format must be restricted by small number of clear and easy-to-follow rules. These rules will ensure full description of the data (physical meaning, units, bibliography etc.) and the cross-referencing if the data comes in several parts. In the end we may support several formats but we start by developing a tool for importing data in form of ASCII tables. This document will also describe a unified DB interface and the methods of tuning it to the existing DBs.
- *Guidelines for the expert quality assessment.* This document will contain a summary of data quality assessment procedures adopted in major existing databases (e.g. VALD, NIST etc.) and a description of the data access protocol, available tools and data usage policy during the assessment period. This document will be revised in the future incorporating the VAMDC own experience, expert comments and suggestions and therefore it must be updated on a regular basis.
- *Selection of an open-source relational database to be used in Path B.* This document will contain a report explaining the motivation behind the selection of specific software.
- *Detailed deployment/verification/maintenance instructions for Path B.* Although the software and the VAMDC interface for Path B will be provided by the WP7, the actual deployment and data publishing must be thoroughly tested before adding a new resource to VAMDC. Both procedures must be described very clearly under the assumption that the data producer does not have special training in installing and running relational databases. A critical requirement for Path B is service availability and sustainability on a long run. These issues will also be addressed by this document.
- *Statistics and data bibliography.* We have identified the lack of proper referencing to the original data producers as the major concern for publishing in large databases. Solving this issue will be a major incentive for the data producer to publish their data through VAMDC. This document should specify the rules for storing and cross-referencing the bibliographic and A&M data as well as the logs of processed requests so any request can be traced back to the source of the extracted data.

Software tools to be developed in WP7:

- VAMDC interface for publishing new A&M data
- Data import tool
- Automatic data verification tool
- VAMDC interface for a selected open source database with the support of VAMDC data exchange protocols
- VAMDC interface for data quality experts (Quality assessment report)

Coordination and Cooperation:

Many of the items to be developed in WP7 are closely related or dependent on other work packages and thus require very close coordination and often collaboration to avoid effort duplication and interface incompatibility. While those questions will be in competence of WP2 we feel that it is our responsibility to identify them. The following specific topics of the WP7 involve interaction with other work packages:

- The format of internal data representation/transport in the VAMDC is critically important for the Data Preparation Rules.
- Guidelines for the quality assessment will be prepared by the WP7 but must be discussed and approved by the VAMDC VPB (WP1 and WP2). See e.g. the point on "quality assurance systems" in Task 1 of WP2 plan for period 1.
- The selection of the open source database and its instrumentation is dependent on both the internal data representation and the registry query protocol adopted in VAMDC. This requires coordination with WP5 and WP6.
- Path B deployment document aimed at data providers must coordinated with WP4 but also with WP3.
- The cross-referencing system and the request logging mechanism must be distributed between individual databases and the VAMDC server. This is as much policy question as it is a technical issue. Thus it must be a cooperation topic with WP2 and WP4.
- The data Import Tool interface to the VAMDC database(s) must comply with the VAMDC internal data representation. This calls for cooperation with the WP6.
- The software package for the Path B must be coordinated with WP4 and WP5.
- Automatic data verification tool overlaps with SA2:T5 of the WP5.
- VAMDC interface will be mostly developed within WP6 but parts of it will be included in WP7 while testing/verification will involve WP4 and WP5.

Coordinating activities will be carried out through systematic updating of the wiki pages, extensive email exchange, use of version control software for the toolkit development and regular working meetings. The following working meetings have been planned for Period 1:

1. Coordination with WP6, Köln, February 2010
2. XSAMS and registry toolkits, Paris, March 2010
3. Automatic registry updates and referencing system within VAMDC, Vienna or Florence, March 2010
4. Test deployment of the VAMDC interface prototype for VALD, Moscow (TBC), May 2010

Here is a description of specific steps within each task planned for Period 1:

Task 1: The current version of the XSAMS will be used is a basis for creating a toolkit for various VAMDC applications. The toolkit will be primarily aimed at data conversion to and

from XSAM to ASCII tables and other formats (April 29th, 2010, Doronin, Nenadovic, Dubernet).

Task 2: A prototype toolkit will be created for collecting exhaustive information about the content of and A&M database, available extraction tools and procedures as well the usage statistics (June 4th, 2010, Doronin, Nenadovic, Dubernet).

Task 3:

- Formulating the requirements for the "standard" VAMDC database software based on the analysis of the structure, content and selection tools of the existing databases (March 1st, 2010, Marquart, Heiter) Note: WP2 Task 1 includes a "census of all VAMDC resources" - the results of this task will be used in WP7/Task 3.
- Finalizing the WP7 plan, internal deliverables and time lines for each partner and writing Publishing Tools Report 1 (April 12th, 2010, Piskunov, Heiter).
- Preparing first version of specification for the format of the data to be imported into VAMDC (April 29th, 2010, Marquart, Piskunov).
- Preparing the prototype of the import tool (together with the RFNC-VNIIT, May 3rd, 2010, Marquart).
- Selection of the "short list" candidates for the VAMDC "standard" database (May 28th, 2010, Marquart, Stempels).
- Testing the import tool with VALD and Spectr W^3 databases (June 11th, 2010, Marquart, Heiter, Stempels).

Task 4: Prototype development and deployment of the VAMDC XSAMS interface for the VALD and Spectr W^3 databases (June 4th, 2010, Marquart, Laboda).

Task 5: A prototype automatic data verification tool developed for a “test” atom and CO-molecule will be created and tested for primary data sources. (May 28th, Fazliev).

- Formulating the requirements for the "standard" middleware based on the analysis of the atomic and molecular data and metadata structures and constructing first version of middleware (June 30, 2010, Akhlyostin)
- Preparing specification for the quantum numbers of CO-molecule, a “test” atom and the corresponding selection rules (March 1st, 2010, Perevalov, Ryabchikova)
- Preparing the prototype of the upload data system for the molecular data (CO-molecule transitions and line profiles data structures) from primary data sources (March 1, 2010, Lavrentiev, Privezentsev).
- Preparing the prototype of the upload data system for the atomic data (the atom transitions and line profiles data structures) from primary data sources (May 1, 2010, Lavrentiev, Privezentsev).
- Preparing the prototype of the tabular presentation system of molecular data (CO-molecule transitions and line profiles data structures) from primary data sources (April 1, 2010, Akhlyostin).
- Preparing the prototype of the tabular presentation system of atomic data (transitions and line profiles data structures) from primary data sources (April 1, 2010, Akhlyostin).
- Formulating the requirements for publication tools (analysis of the relations between the data owner and person reviewing the data). Preparing specification of these relations and prototype of the software implementing the publishing procedure. (May 28, 2010, Kozodoev)

Release of the software, documentation, test results, performance assessment and procedure documents for Tasks 1-5 will be available through links from the VAMDC web-site.

13. WP8 ACTIVITIES DESCRIPTION

WP8 is JRA3: New mining and Integration Tools

13.1 WP8 Objectives

This JRA will develop extensions to the baseline infrastructure. Key objectives are the design of advanced data mining tools and the design of cross-matching and cross-federating tools, providing sophisticated integrated science services aimed at maximising the scientific utility to the end user community of the VAMDC services.

WP8 Leader is UCL(3)

13.2 WP8 Milestones and Deliverables

Milestones

M8.1	Technical Meetings	WP8	UU	Months 5,10, 16, 22, 28, 34, 40, 42	Minutes. Presentations on internal Website
M8.2	Evaluation of softwares	WP8	UU	Months 10, 22, 34	

Deliverables

D8.1 Mining and Integration Tools Plan (PM 3)
D8.2 Mining and Integration Tools Report to be included in report to the EU – Year 1 (PM 10)
D8.3 Mining and Integration Tools Report to be included in report to the EU – Year 2 (PM 22)
D8.4 Mining and Integration Tools Report to be included in report to the EU – Year 3 (PM 34)
D8.5 Final Report of Mining and Integration Tools to be included in final report to the commission (PM41)
Annual Mining & Integration Plan revisions included in Revised Annual VAMDC Project Plans – Year 1,2,3

13.3 WP8 Tasks Description

WP8 Leader (co)		
Task Number	Leader	Other Partners
1	M. Doronin (CNRS: LPMAA)	RFNC-VNIITF
2	S. Schlemmer (KOLN)	CNRS:LPMAA
3	J. Tennyson (UCL)	UCL/MSSL

Description of work (possibly broken down into tasks)

Through the activities of JRA1 and JRA2, the AM resources will be searchable and will provide information in a standardised way. The following step is to build the query protocols

that will access those published AM data and then to design software that will handle and process those data.

Task1: Registry Queries (lead by CNRS(1) with (12))
We will need to use protocols to query the registries at a fine level of granularity. Indeed we don't wish to only find resources having implemented a type of service such as SSAP or TAP, but rather be able to select resources according to their content through key words. The purpose of Task 1 is to implement those protocols.

Task 2: Tools for Manipulation of Data (lead by KOLN(7) with (1))
Our queries will return data organised according to schemas defined in JRA1. Those schemas will be quite complex because they will reproduce all the scientific concept attached to the data. Therefore the handling of the XML files will be complex and will require specific tools. For now we identify too main generic tools: one performing cross-matching of data and one performing cross-federation of data. These tools are particularly difficult because they require to compare the content of many fields in the schema. Those generic tools will be made available for download in SA1 to the end users and developers. Support to adapt those tools to specific applications will be provided in SA2. We plan to provide libraries to allow users to develop their own applications

Task 3: VAMDC advanced data mining services (lead by UCL(3))
With the deployment of a vast range of high value data services through the standard VAMDC infrastructure, this task will investigate optimal strategies to best mine these AM data resources to both advance the creation of new AM fundamental data, and by providing stream lined automated access to appropriate AM data targeted at specific user groups (for the astronomy community benefiting from the availability of high energy data from satellites such as Swift, XMM, Chandra, who require specific atomic data for high excitation species of elements such as iron). This task would investigate the provision of application services wrapping complex work flows combining AM data access, manipulation, and integration into user processing chains – e.g. in solar physics, astro-biology/ chemistry and so forth.

13.4 WP8 Tasks Description for Period 1

Full task activities are detailed at the VAMDC wiki on the WP8/JRA3 pages – see http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/WP8

Task 1: Registry Queries

- This task is not due to start until Cycle 2

Task 2: Tools for Manipulation of Data

- Make Prototype of Data cross-identification software based on current XSAMS schema (link with JRA1/JRA2) – Initial Test for Cycle 1 will be between BASECOL and CDMS databases.

Task 3: VAMDC advanced data mining services

- Development of use cases for workflows based around e-HITRAN

- Identify current and future users/data miners of the HITRAN database and its upcoming successor, e-HITRAN
- Survey the current and future HITRAN/e-HITRAN users as to how they do/would mine the information contained in the database
- Develop a series of use cases based upon the responses of users

- Development of technical requirements of workflows
  - Begin dialogue with MSSL on the technical requirements for workflows to support the use cases

14. EFFORT DISTRIBUTION

Project number (acronym) : VAMDC - **239108**

First line is EC requested staff months of effort whilst the second line for each partner in () is number of contributed staff months of effort.

Partner number	Short Name	WP1 MGT	WP2 NA1	WP3 NA2	WP4 SA1	WP5 SA2	WP6 JRA1	WP7 JRA2	WP8 JRA3	Total PM Per Beneficiary
1	CNRS	15 (15)	6 (6)	0 (6)	33 (33)	27 (27)	18 (18)	6 (6)	6 (6)	111 (117)
2	CMSUC	0 (2)	3 (6)	9 (0)	18 (18)	18 (18)	0 (0)	0 (0)	0 (0)	48 (44)
3	UCL	0 (2)	3 (6)	3 (0)	18 (18)	12 (12)	0 (0)	0 (0)	18 (18)	54 (56)
4	OU	0 (2)	0 (2)	9 (9)	6 (6)	0 (0)	0 (0)	0 (0)	0 (0)	15 (19)
5	UNIVIE	0 (2)	0 (0)	8 (6)	3 (3)	0 (0)	0 (0)	0 (0)	0 (0)	11 (11)
6	UU	0 (2)	3 (3)	6 (2)	3 (3)	0 (0)	9 (9)	6 (6)	0 (0)	27 (25)
7	KOLN	0 (2)	3 (3)	1 (0)	4 (4)	0 (0)	5 (5)	0 (0)	8 (10)	21 (24)
8	INAF-OAC	0 (2)	0 (0)	0 (0)	9 (2)	3 (0)	3 (2)	8 (4)	0 (0)	23 (10)
9	QUB	0 (2)	3 (3)	0 (0)	0 (0)	0 (0)	6 (6)	0 (0)	0 (0)	9 (11)
10	AOB	0 (2)	0 (0)	6 (6)	0 (0)	0 (0)	3 (3)	0 (0)	0 (0)	9 (11)
11	ISRAN	0 (2)	0 (0)	0 (0)	0 (0)	9 (9)	0 (0)	0 (0)	0 (0)	9 (11)
12	RFNC-VNIITF	0 (2)	0 (0)	0 (0)	5 (0)	0 (5)	1 (2)	3 (2)	3 (3)	12 (14)
13	IAO	0 (2)	0 (0)	3 (3)	6 (3)	3 (3)	0 (0)	12 (12)	0 (0)	24 (23)

14	CPTM	0 (2)	3 (3)	8 (3)	18 (6)	0 (0)	3 (3)	0 (0)	0 (0)	32 (17)
15	INASAN	0 (2)	3 (3)	3 (0)	0 (0)	6 (6)	0 (0)	0 (0)	0 (0)	12 (11)
Total: EU+ Contributed	Staff months	58	62	91	219	158	96	65	72	821

15. ESTIMATED BUDGET BREAKDOWN PER WORK PACKAGE FOR THE WHOLE PERIOD (42 MONTHS)

Following the **budget requested** to EU (and not the eligible costs) indicated in the Grant Agreement Preparation Forms from the 28-05-2009, which is in accordance with the budget breakdown indicated in Annexe B of the Grant Agreement, we can estimate the following breakdown of budget per workpackage:

	RTD	Coordination	Management	Others
WP1			187200	
WP2		238400		
WP3		349910		
WP4				877895
WP5				633368
WP6	252660			
WP7	171071			
WP8	189495			
TOTAL	613227	588310	187200	1511263

The estimated % for total requested EC contributions for Period 1 (Month 1 to 12) is about 24%, for Period 2 and 3 (each period is 12 months) are about 31% each, for last period (Month 37 to 42) is about 14%. The estimated breakdown per WP and per period can be obtained applying those coefficients to the above table.