VAMDC AS A RESOURCE FOR ATOMIC AND MOLECULAR DATA AND THE NEW RELEASE OF VALD

F. Kupka\(^1\) and the VAMDC Collaboration (P.I. M.-L. Dubernet)\(^2,3\)

\(^1\) Faculty of Mathematics, University of Vienna, Nordbergstraße 15, A-1090 Vienna, Austria; Friedrich.Kupka@univie.ac.at
\(^2\) LPMAA, UMR7092 CNRS/INP, Université Pierre et Marie Curie, France; Marie-Lise.Dubernet-Tuckey@upmc.fr
\(^3\) LUTH, UMR8102 CNRS/INSU, Observatoire de Paris, France

Received: ???; accepted: ???

Abstract. The Virtual Atomic and Molecular Data Centre (VAMDC) (M.L. Dubernet et al. 2010, JQSRT 111, 2151) is an EU-FP7 e-infrastructure project devoted to building a common electronic infrastructure for the exchange and distribution of atomic and molecular data. It involves two dozen teams from six EU member states (Austria, France, Germany, Italy, Sweden, United Kingdom) as well as Russia, Serbia, and Venezuela. Within VAMDC scientists from many different disciplines in atomic and molecular physics collaborate with users of their data and also with scientists and engineers from the information and communication technology community. In this presentation an overview of the current status of VAMDC and its capabilities will be provided. In the second part of the presentation I will focus on one of the databases which have become part of the VAMDC platform, the Vienna Atomic Line Data Base (VALD). VALD has developed into a well-known resource of atomic data for spectroscopy particularly in astrophysics. A new release, VALD-3, will provide numerous improvements over its predecessor. This particularly relates to the data contents where new sets of atomic data for both precision spectroscopy (i.e., with data for observed energy levels) as well as opacity calculations (i.e., with data involving predicted energy levels) have been included. Data for selected diatomic molecules have been added and a new system for data distribution and data referencing provides for more convenience in using the upcoming third release of VALD.

Key words: atomic data – molecular data

1. INTRODUCTION

The Virtual Atomic and Molecular Data Centre (VAMDC) has been founded to develop an interoperable electronic infrastructure for the exchange of atomic and molecular data. It unites 15 administrative partners who represent 24 teams from six European Union member states (Austria, France, Germany, Italy, Sweden, United Kingdom) as well as the Russian Federation, Serbia, and Venezuela. Scientists from a wide variety of disciplines in atomic and molecular physics are
involved in VAMDC as well as scientists and engineers from information and communication technology. Since many partners of VAMDC have already developed specialized data bases in their own field and many of them maintain a close connection to both data producer and data user communities, these resources were a natural asset of VAMDC from its very beginning.

The key difference of VAMDC to the databases provided by any of its contributors is that the newly developed electronic infrastructure allows access to each of these data resources through a single portal. The effort required by users in finding and retrieving data can thus be minimized, while the data sets themselves become available to a much wider community.

One of the databases integrated into the VAMDC framework is VALD, the Vienna Atomic Line Data Base (Piskunov et al. 1995, Kupka et al. 1999, Ryabchikova et al. 1999, Heiter et al. 2008). Developed and maintained at three of the VAMDC partner institutions, VALD has served as one of the databases selected for prototype implementations of VAMDC. The data collection available to VALD has been greatly enhanced as a result of very close collaboration with data producers. Through the development of VAMDC new functionality has been added. This new release, denoted VALD-3, has now reached a state of development which soon will permit its official distribution to the user community.

In the following section, the main concepts and capabilities of VAMDC are described. Its current status and further development plans are then reviewed. Finally, the most important improvements of VALD-3 over previous releases are briefly described. A final section summarizes these developments and looks forward to new releases of VAMDC.

2. CONCEPTS AND CAPABILITIES OF VAMDC

Atomic and molecular data have been collected and assessed in various databases which underpin a wide range of physics in applied research and industrial development. Many of them have been built to serve specific needs. VALD is one such example with its own advantages, special tools, and limitations. Heterogeneous data sets have been collected in different formats and with a varied degree of completeness. Specialized extraction tools exist for most of the databases, which often significantly contribute to their popularity. However, this development has also created problems: data often exist in duplicated form, sometimes also within a database, which requires non-trivial selection criteria when using them. Moreover, different user interfaces have to be handled each time a different database is being accessed. Thus access may be restricted and the available data may be fragmentary as a result of the collection process.

The main outcome expected from the VAMDC project is to

- develop and extend standards for interoperability of resources on atomic and molecular data;
- implement its concepts for selected databases;
- allow easy access to a myriad of data resources;
- query those resources with dedicated protocols and query languages;
- allow asynchronous transfer of large amounts of data;
• create a safe environment for publishing the latest sets of atomic and molecular data;
• link data producers more closely with data users.

The key benefits expected from using VAMDC are the possibilities to
• find any type of atomic and molecular data with a single click;
• have uniform access to the published data;
• allow cross matching of different data sets;
• allow wide access to latest published data.

VAMDC clientele include people working in the fields of astrophysics, astronomy, planetary science, atmospheric science, fusion science, plasma science, the radiation sciences and in the application of such research in e.g. industrial development, for instance, in the lighting industry.

The data exchange with databases that are part of VAMDC is organised through a web-based transport protocol. A user interface and an automatic interface are supported. This also allows access of the data through procedures developed for the international virtual observatory (Quinn et al. 2004). Publishing tools of data producers can access the system in a similar fashion. Mirroring and synchronization of the capabilities developed within VAMDC ensures a highly reliable service. This is backed up by an archiving strategy for long-term preservation of the distributed contents.

The transport protocol of VAMDC handles database queries for the status and data content (registry update), the query and data transfer between the user and the VAMDC portal as well as between specific databases and the portal. The transport protocol is self-descriptive (XML description of the data sent including units, formats etc. based on an extension of the XSAMS data format of Dubernet et al. 2009). It is also efficient for large data sets through using compressed binary tables. The interface to each database is fully compatible with the VAMDC transport on the outside (i.e. how the data resource is seen by a VAMDC user), but tuned to the specific database on the inside (i.e. how VAMDC sees a data resource). Functionalities of this interface include converting incoming queries to the internal query format and converting the database extraction to the transport-compatible VAMDC output format. Further capabilities are the ability to respond to VAMDC-specific queries such as registry updates (to keep track of which resources are available at what location) and collecting accounting information.

For a more detailed discussion of the scope of the VAMDC project the reader is referred to Dubernet et al. (2010) and to http://www.vamdc.eu/.

3. STATUS AND DEVELOPMENT OF VAMDC

An overview on the “Level 1 Release” of VAMDC has been provided by Rixon et al. (2011). Achievements during this period included first prototypes of the protocol and XSAMS data model which were used to develop and provide archive-data services for a small selection of databases: VALD (Piskunov et al. 1995, Kupka et al. 1999, Ryabchikova et al. 1999, Heiter et al. 2008), XstarDB (Bautista
Table 1. Databases accessible through the VAMDC Level 2 Release registry browser. Further information include the VAMDC node hosting the database, and its availability (all databases including those in preparation (in prep.) will become accessible at the most recent portal level). References to the original description are listed in column 5.

| database          | node             | status     | portal | reference                  |
|-------------------|------------------|------------|--------|----------------------------|
| BASECOL           | LPMAA            | available  | level 2| Dubernet et al. 2006       |
| CDMS              | Köln             | available  | level 2| Müller et al. 2005         |
| CDSD              | IAO (LTS) Russia| available  | level 2| Perevalov & Tashkun 2008   |
| CHIANTI           | Cambridge / MSSL | available  | level 2| Dere et al. 2009           |
| Ethylene          | Reims            | available  | level 2| see SkMPO and vadmc.eu     |
| HITRAN            | UCL              | available  | level 2| Rothman et al. 2009        |
| UDIA (UMIST)      | Manchester / QUB (Belfast) | available | level 2| Woodall et al. 2007       |
| VALD              | Uppsala University (mirror) | available | level 2| see text                   |
| GhoSST            | Grenoble         | available  | level 1| Schmitt et al. 2009        |
| Lund data         | Uppsala University | available | level 1| various                    |
| Methane lines     | Dijon            | available  | level 1| see SkMPO and vadmc.eu     |
| SkMPO             | Reims            | available  | level 1| Mikhailenko et al.         |
| Spectr-W³         | RFNC–VNIITF      | available  | level 1| Faenov et al. 2002         |
| KIDA              | Bordeaux         | in prep.   |        | kida.obs.u-bordeaux1.fr    |
| Stark-B           | Paris-Meudon     | in prep.   |        | Jevremovic et al. 2009     |
| TipTopBase        | IVIC / Cambridge | in prep.   |        | Cunto et al. 1993          |

and Kallman 2001), BASECOL (Dubernet et al. 2006), and CDMS (Müller et al. 2005).

Subsequently, protocols and data models have been further refined and a test web-site has been set up with a registry browser which enables users to access data contents from a much larger number of databases. In Table 1 we list the databases included in the level 2 release of VAMDC which are accessible through the registry browser at the time of writing this paper and further databases for which access is just being prepared. All of them are expected to be available upon completion of the level 2 release. Work on further databases is in progress.

Detailed references concerning these databases can be found in Dubernet et al. (2010) and also on the VAMDC web site (http://www.vamdc.eu/), the Wiki page of VAMDC (http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/WebHome), and the VAMDC newsletter available through these resources. After the Level 2 release a larger user community will be invited to test the VAMDC portal and its capabilities and the feedback will be used to improve the final release.

4. IMPROVEMENTS IN VALD–3

VALD was created by an international team of researchers (Piskunov et al. 1995, Kupka et al. 1999, Ryabchikova et al. 1999, Heiter et al. 2008). A lot of its early development occurred during small workshops at the Institute for Astronomy at the University of Vienna which became the site of the main server with mirror sites of the database installed at Uppsala University and the Institute of Astronomy of the Russian Academy of Sciences in Moscow. Today most of the software development and work on integrating molecular data into VALD is performed at Uppsala University. Most of the atomic data collection and systematic testing of the data distributed through VALD occurs at the Institute of Astronomy of the Russian Academy of Sciences in Moscow.

Ahead of the VALD-3 release, the database contains over 160 line lists and over 66 million atomic lines provided by all major spectroscopy centres across the
VAMDC as a resource and the new release of VALD

world. The mirror sites in Vienna, Uppsala, and Moscow serve nearly 1500 users from more than 50 countries. On average 30 requests are being processed per day.

VALD was designed to compile accurate and complete line lists for stellar atmospheres and spectroscopy. Line lists included within it are evaluated to provide a ranking which is used to prefer in the case of duplicated entries one set of data over another. The database was designed to be expandable with respect to data and content to allow simple access through customized extraction software, fast access to individual data entries, and allow either an overview of parameters from different sources or, as an alternative choice, extract sets of the best available data according to data ranking lists and compile data references for citing original sources.

To this end before adding a data set to the database the data have to be converted first into a standard format with units which are commonly used in astrophysics. Multiple extraction layers within VALD allow accessing and merging of the data and prepare output for different applications. Requests can be posed as e-mails or issued through a web interface. Originally data were sent back only by e-mail, although as part of VALD-3 a possibility for downloading much larger responses to user requests will be offered (internally, data output can simply be streamed into files or standard text input interfaces).

Several quantities must be known about a line when adding its data to VALD: central wavelength, species identifier, log$(gf)$, and energies as well as total angular momentum quantum numbers of lower and upper levels of the transition. These are the most crucial data for calculating absorption lines (in local thermal equilibrium) and they are also used for deciding on how to merge line lists from different sources. Lines are considered to be identical, if they originate from the same species, have identical total angular momentum quantum numbers for both levels and differ by less than a threshold with respect to wavelength and energy of both levels.

Further data entries which can be added for a spectral line included within the VALD database are Landé-factors of both energy levels, damping constants for natural line broadening as well as quadratic Stark effect and Van-der-Waals broadening, term designations, and information on accuracy or comments on multiplets, as well as some multipurpose flags.

For spectral lines where both energy levels are experimentally known the mandatory data entries are usually sufficient to uniquely distinguish them and avoid erroneous identification of duplicates. Since lines with at least one predicted energy level have a very low ranking, such data will be rejected, when misidentified with a spectral line with observed energy levels, which results in the worst case in putting out a (usually very weak) predicted line. No false information can be generated this way in an entry put out as a response to a request to the database. Such a potential loss only affects statistical opacity calculations for model atmospheres, since for precision spectroscopy data with even just one predicted energy level is useless because of an unacceptable uncertainty in wavelength of the transition. It is important to note here that also term designations may be uncertain for some spectral lines and that their notation can be incoherent among different sources. Hence, using them as an additional criterion for line identification was not an option when VALD was originally created. The introduction of such a consistent notation for the line data stored is still an ongoing project.

The ranking provided by the VALD team uses quality determinations based on error estimates from original sources, comparisons with existing alternative
sources, and applications in astrophysics (user feedback). A re-ranking is possible and has occurred on several occasions. General guidelines for this process are that experimental data are preferred over calculations (with few exceptions) and data with individual error estimates are considered more reliable. Line lists from homogeneous sources with high accuracy data are given priority over sources which are inhomogeneous or have low quality data. To add flexibility to this process users can change the ranking for the merging process.

While the first two releases of VALD, dating from 1995 and 1999 (with a subsequent number of data updates) were accomplished by a rather small team of researchers, the VALD-3 release is now being prepared by a much larger group which is a consortium of scientists from different institutions. Already the core group working in Uppsala, Moscow, and Vienna is twice as large and includes U. Heiter, N. Piskunov, H.C. Stempels as well as P. Barklem and O. Kochukhov at Uppsala University, R. Kildiyarova, Yu. Pakhomov and T. Ryabchikova at Institute of Astronomy of the Russian Academy of Sciences in Moscow, with both sides supported by further researchers working primarily on VAMDC, and F. Kupka, T. Rank-Lüftinger, W.W. Weiss at University of Vienna, where further researchers have contributed to earlier stages of VALD-3 (L. Fossati, N. Nesvacil, M. Obbruger, Ch. Stütz). There is also a very close collaboration with many of the leading data producers in the area of interest for VALD. This originally included the spectroscopy group at the University of Wisconsin headed by J.E. Lawler and E.A. Den Hartog, the spectroscopy group at Lund University (H. Nilsson et al.), the Dream Database team (Biémont et al. 1999), as well as B. Plez at the Université de Montpellier and R.L. Kurucz at CfA in Harvard, the team of J.S. Sobeck et al. at the University of Texas at Austin, and the team at Imperial College London, headed by J.C. Pickering and R.J. Blackwell-Whitehead. The list of data provides is still growing at this point.

In VALD-3, data are still sorted as a function of wavelength and still stored in a special compressed format allowing semi-direct access to individual entries. The data stored therein still contains for each spectral line a species description, wavelength (inside the database consistently in Å for vacuum conditions), energies of lower and upper levels (now in cm$^{-1}$), total angular momentum quantum number, oscillator strength in the form of log $gf$, Landé-factors of both energy levels, damping constants, but also more information on the accuracy of log $gf$, and in addition to the data reference, a full designation of level and term name.

Publishing a new data set in VALD-3 still means adding a new data file to the existing set, while data description continues to be stored in various support files (i.e., a list of species, and a configuration file which stores ranks for every field in each file to allow merging data from different sources). An important change is that references for each data set are now provided in BibTeX format. Indeed, the origin of each entry is now accessible even for merged line lists such as BELLHEAVY (cf. Kurucz 1992).

In addition to many smaller new lists the New Kurucz Calculations (2006-2010) for Fe-peak elements have been included into the data. All these additions allow much more accurate matching of absorption line spectra of various types of stars. The model-based selection of lines within VALD, a very popular tool among users, has also been improved to make estimates of the contribution to opacities and predictions of the line strength more accurate and convenient.
5. OUTLOOK AND CONCLUSIONS

In spite of its improvements the upcoming VALD-3 release is subject to a number of restrictions: the range of ionization stages is limited (neutral up to 8 times ionized) and only simple molecules will be included in VALD-3 (basically diatomics: TiO, CO, CN, CH, C$_2$, FeH). Generally missing data include collisional transition probabilities and advanced broadening approximations, among others. Since the VALD consortium has neither the personnel nor the expertise to fix these deficiencies, even frequent VALD users may sometimes want to look for alternatives. One possible solution is to access the VAMDC data resources.

With its very wide range of atomic and molecular databases VAMDC can offer a common access portal to a large variety of data collections through platform and database independent methods. It thus can provide benefits for both current users of the databases participating in VAMDC and to novice users searching for information on atomic and molecular data who will no longer have to learn how to use a multitude of interfaces.

A number of conferences will provide opportunities for testing VAMDC and also offer tutorials on how to use its capabilities. The third annual VAMDC Conference which will take place in Vienna, Austria, from 21-24 February 2012 (see [http://www.vamdc.eu/]) is one such opportunity, as is the VAMDC Regional Workshop and School in Atomic and Molecular Data, which is to take place in Belgrade, Serbia, from 7-9 June 2012 ([http://poincare.matf.bg.ac.rs/~andjelka/VAMDC/]). It is hoped that in the future VAMDC will become the reference location in the internet where to look for atomic and molecular data.

ACKNOWLEDGMENTS. F. Kupka would like to express his gratitude to the LOC of the 8th SCSLSA for financial support as well as the Austrian FWF for funding through project P21742-N16. The help and suggestions of U. Heiter and N. Mason who carefully proofread this manuscript are greatly appreciated. This work has been presented as part of the VAMDC collaboration. VAMDC is funded under the “Combination of Collaborative Projects and Coordination and Support Actions” Funding Scheme of The Seventh Framework Program. Call topic: INFRA-2008-1.2.2 Scientific Data Infrastructure. Grant Agreement number: 239108.

REFERENCES

Bautista, M.A., Kallman, T.R. 2001, Astrophys. J. Suppl. 134, 139
Biémont, E., Palmeri, P., Quinet, P. 1999, Astrophys. J. Suppl. 635, 2691
Cunto, W., Mendoza, C., Ochsenbein, F., Zeippen, C. 1993, A&A 275, L5
Dere, K.P., Landi, E., Young, P.R. et al. 2009, A&A 498, 915
Dubernet, M.L., Grosjean, A., Flower, D. et al. 2006, Ro-vibrational Collisional Excitation Database BASECOL ([http://basecol.obspm.fr/]), in Proceedings of the Joint Meeting ITC14 and ICAMDATA 2004, Tohoku, Japan. J. Plasma Fusion Res. Ser. 7, 356
Dubernet, M.L., Humbert, D., Clark, R.E.H. et al. 2009, XSAMS: XML schema for Atomic, Molecular and Solid Data. In: Dubernet, M.L., Humbert, D., Ralchenko, Yu., editors. [http://www-amdis.iaea.org/xml/]. Version 0.1, September 2009.
Dubernet, M.L., Boudon, V., Culhane, J.L. et al. 2010, Jour. Quant. Spectr. Rad. Transfer, 111, 2151
Faenov, A.Y., Magunov, A.I., Pikuz, T.A. et al. 2002, Spectr-W-3 online database on atomic properties of atoms and ions. AIP Conf. Proc. 636, 253
Heiter, U., Barklem, P., Fossati, L. et al. 2008, VALD – an atomic and molecular database for astrophysics, Journal of Physics Conference Series 130, 1
Jevremović, D., Dimitrijević, M.S., Popović, L.Č et al. 2009, New Astron. Rev. 53, 222
Kupka, F., Piskunov, N., Ryabchikova, T.A. et al. 1999, A&A Suppl., 138, 119
Kurucz, R.L. 1992, Rev. Mex. Astron. Astrof. 23, 45
Mikhailenko, S., Barbe, A., Babikov, Y., Tyuterev, V.G. S&MPO a databank and information system for ozone spectroscopy on the WEB, ⟨http://smpo.iao.ru/⟩.
Müller, H.S.P., Schlöder, F., Stutzki, J., Winnewisser, G. 2005, J. Mol. Struct. 742, 215
Perevalov, V.I., Tashkun, S.A. 2008, CDSD-296 (Carbon Dioxide Spectroscopic Databank): updated and enlarged version for atmospheric applications. In: 10th HITRAN database conference, Cambridge, MA, USA; fourth assessment report of the intergovernmental panel on climate change. Cambridge, UK: Cambridge University Press.
Piskunov, N.E., Kupka, F., Ryabchikova, T.A. et al. 1995, A&A Suppl., 112, 525
Quinn, P., Barnes, D., Csabai, I. et al. 2004, The International Virtual Observatory Alliance: recent technical developments and the road ahead, SPIE 5493, 137
Rixon, G., Dubernet, M.L., Piskunov, N. et al. 2011, in 7th International Conference on Atomic and Molecular Data and Their Applications – ICAMDATA–2010, AIP Conf. Proc. 1344, 107
Rothman, L.S., Gordon, I.E., Barbe, A. et al. 2009, JQSRT 110, 533
Ryabchikova, T.A., Piskunov, N.E., Stempels, H.C., et al. 1999, in Proc. of the 6th Int. Coll. on Atomic Spectra and Oscillator Strengths, Victoria BC, Canada, Phys. Scripta, T83, 162
Schmitt, B.P., Volcke, E., Quirico, O. et al. 2009, GhoSST: the Grenoble astrophysics and planetology solid spectroscopy and thermodynamics database service: RELEVANT Database, see ⟨http://ghostt.obs.ujf-grenoble.fr/⟩.
Woodall, J., Agúndez, M., Markwick-Kemper, A.J., Millar, T.J. 2007, A&A 466, 1197