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# A Decade with VAMDC: Results and Ambitions

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1 **Abstract:** This paper presents an overview of the current status of the VAMDC e-infrastructure  
2 including the current status of the VAMDC connected (or to be connected) databases, updates on the  
3 latest technological development within the infrastructure and a presentation of some application  
4 tools that make use of the VAMDC e-infrastructure. We analyse the past 10 years of VAMDC  
5 development and operation, and assess their impact both on the field of atomic and molecular  
6 (A&M) physics itself and on heterogeneous data management in international cooperation. The  
7 highly sophisticated VAMDC infrastructure and the related databases developed over this long term  
8 make them a perfect resource of sustainable data for future applications in many fields of research.  
9 However, we also discuss the current limitations that prevent VAMDC from becoming the main  
10 publishing platform and the main source of A&M data for user communities, and present possible  
11 solutions under investigation by the consortium. Several user applications examples are presented,  
12 illustrating the benefits of VAMDC in current research applications, which often need the A&M data  
13 from more than one database. Finally, we present our vision for the future of VAMDC.

14 **Keywords:** scientific databases; atomic and molecular data; interoperability; FAIR principles; open  
15 access

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## 16 1. Introduction

17 The Virtual Atomic and Molecular Data Centre (VAMDC) has been developed to interconnect  
18 atomic and molecular databases, thus providing a single location where users can access atomic and  
19 molecular (A&M) data. The VAMDC portal currently provides access to 38 databases containing a  
20 wide range of data from atomic spectroscopy (VALD, section 2.1.2) to PAH theoretical data (PAH,

21 section 2.2.2). The paper presents the current status of the VAMDC project and its underlying databases,  
22 and gives some examples of the exploitation of VAMDC by some exemplar user communities; we  
23 describe open issues in the project and our vision for future developments.

24 The VAMDC project<sup>1</sup> originated as a European Union framework 7 (FP7) research infrastructure  
25 project [1] that was funded between 2009 and 2012, and subsequently extended through the  
26 SUP@VAMDC project<sup>2</sup> [2] between 2012 and 2014. Since 2014 the VAMDC Consortium has operated as  
27 an independent body comprising some 35 research groups. This consortium has continued to operate  
28 and develop the data centre, as well as pursuing other related objectives in data science. The VAMDC  
29 consortium published its original aims in 2010 [1], which were updated in 2016 following the formal  
30 launch of the independent consortium [3]. The public entry of the VAMDC consortium is its public  
31 website<sup>3</sup> that provides an access to data and documentation, as well as consortium-related information  
32 such as current membership and how to join us<sup>4</sup>.

## 33 2. Current Status of VAMDC Connected Databases

34 The VAMDC nodes are distributed such that they are located at the members' and partners' sites.  
35 At present most of the databases included in the VAMDC e-infrastructure are databases used primarily  
36 in astrophysics. The common output format is the XML Schema for Atoms, Molecules and Solids  
37 (XSAMS) (see section 3.1.1) that uses the tree-structured form of the data model. All of the current  
38 VAMDC databases are listed on the VAMDC portal<sup>5</sup> which also provides a short introduction to the  
39 database, a link to its public graphical interface and contact details of a member of that database team  
40 to whom inquiries may be directed. In addition, it is possible to list the atoms and the molecules that  
41 can be queried from those databases.

42 Table 1 provides a summary of the 38 databases currently accessible via VAMDC. It includes eight  
43 databases that are in the process of joining the consortium. It should be noted that a database might be  
44 off-line for a period of time due to maintenance issues.

45 Among the databases already present in the VAMDC e-infrastructure in 2016 and cited in our  
46 last publication [3], some have evolved with respect to their data content, functionalities and internal  
47 structure, and improved their interoperability with the VAMDC ecosystem. Some of them have not  
48 evolved, and two have been disconnected from the VAMDC ecosystem. Ten databases have been  
49 added. Among these new databases is a new node at NIFS in Japan.

### 50 2.1. Evolution of VAMDC Nodes/Connected Databases since 2016

51 Each individual database incorporated in VAMDC will now be discussed highlighting recent  
52 developments and improvements.

#### 53 2.1.1. NIFS Databases

54 The National Institute for Fusion Science (NIFS) has compiled and developed an extensive atomic  
55 and molecular numerical database on collision processes which has been open for public access<sup>6</sup>  
56 since 1997. A data compilation on collisional cross sections for hydrogen, its isotopes and helium  
57 [41,42] was initiated by a collaborative working group of atomic and plasma researchers from Japanese  
58 universities, organised at the Institute of Plasma Physics, Nagoya University, in 1973. Subsequent  
59 compilations were published in IPPJ-AM reports in 1977–1989 and as NIFS-DATA reports since 1989

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1 <http://www.vamdc-project.vamdc.eu/>

2 <http://www.sup-vamdc.vamdc.org/>

3 <http://www.vamdc.org>

4 <http://www.vamdc.org/structure/how-to-join-us/>

5 [https://portal.vamdc.eu/vamdc\\_portal/nodes.seam](https://portal.vamdc.eu/vamdc_portal/nodes.seam)

6 <http://dbshino.nifs.ac.jp>

**Table 1.** Table of databases connected to VAMDC (C) and to be connected (TC). User fields are labelled as follows for applications in astrophysics and planetary science: stellar physics (STEL), solar physics (SOL), interstellar medium (ISM), earth (E), planets (PL), exoplanets (EXO), brown dwarfs (BDW), comets (C). Partnerships are indicated as Full Members (FM) according to the VAMDC Consortium MoU and partners following the VAMDC technical quality chart only (P).

Database	Data Classification	Applications
NIFS Database <sup>c</sup>	atomic, molecular processes [4,5]	STEL, SOL, plasma, fusion
VALD <sup>b</sup>	atomic, molecular linelists [6]	STEL, SOL
VALD-Moscow <sup>b</sup>	atomic, molecular linelists [6]	STEL, SOL (subset) 2.1.2
NIST ASD <sup>c</sup>	atomic lineslists [7]	STEL, ISM
Spectr-W <sup>3 c</sup>	atomic lineslists and collisions [8]	STEL, SOL, plasma, fusion
CHIANTI <sup>b</sup>	atomic lineslists and collisions [9]	SOL
TIPbase <sup>b</sup>	atomic linelists and collisions [10]	STEL, SOL, plasma
TOPbase <sup>b</sup>	atomic linelists and collisions [11]	STEL, SOL, plasma
Stark-B <sup>b</sup>	atomic line shifts, broadening [12,13]	STEL, plasma
CDMS <sup>b</sup>	molecular linelists [14]	ISM, E, C
JPL <sup>c</sup>	molecular linelists [15]	ISM, E, C
HITRAN <sup>c</sup>	molecular linelists, broadening coefficients [16]	E, PL, EXO
S&MPO <sup>b</sup>	O <sub>3</sub> linelists [17]	E, EXO
MeCaSDa <sup>b</sup>	CH <sub>4</sub> linelists [18]	E, EXO, PL, DBW
ECaSDa <sup>b</sup>	Ethene calculated linelists [18]	E, PL
TFMeCaSDa <sup>b</sup>	Tetrafluoro-Methane calculated linelists [18]	E
SHeCaSDa <sup>b</sup>	Sulfur Hexafluoride calculated linelists [18]	E
GeCaSDa <sup>b</sup>	GeH <sub>4</sub> linelists [18]	PL
RuCaSDa <sup>b</sup>	RuO <sub>4</sub> linelists [18]	Nuclear industry
TFSiCaSDa <sup>b</sup>	SiF <sub>4</sub> linelists [18,19]	E
UHeCaSDa <sup>b</sup>	UF <sub>6</sub> line lists ( <sup>a</sup> )	Nuclear industry
CDS-296 <sup>b</sup>	CO <sub>2</sub> linelists [3,20]	E, PL, EXO, BDW
CDS-1000 <sup>b</sup>	CO <sub>2</sub> linelists [3]	E, PL, EXO, BDW
CDS-4000 <sup>b</sup>	CO <sub>2</sub> linelists [21]	E, PL, EXO, BDW
NOSD-1000 <sup>b</sup>	N <sub>2</sub> O linelists [22]	E, PL, EXO
NDSD-1000 <sup>b</sup>	NO <sub>2</sub> linelists [23]	E, PL, EXO
ASD-1000 <sup>b</sup>	C <sub>2</sub> H <sub>2</sub> linelists [24]	E, PL, EXO
SESAM <sup>b</sup>	VUV small molecules linelists [13]	ISM, STELL
W@DIS <sup>b</sup>	atmospheric molecule data sources [25]	E, PL
KIDA <sup>b</sup>	chemical kinetics [26,27]	ISM, PL
UDfA <sup>b</sup>	chemical kinetics [28]	ISM, PL
BASECOL <sup>b</sup>	molecular collisions [29,30]	ISM, C
MOLD <sup>b</sup>	photo-dissociation cross sections [31,32]	STEL
BeamDB <sup>c</sup>	molecule/atom-electron cross-sections [33]	Plasma, radiation damage
IDEADB <sup>c</sup>	dissociative electron collisions [34]	PL, EXO, ISM, radiation damage
GhoSSt <sup>b</sup>	solid spectroscopy data [35]	ISM, PL
LASp <sup>b</sup>	solid spectroscopy data [3]	ISM, PL
PAH <sup>b</sup>	PAH theoretical Data [3,36]	ISM, PL, E
ExoMolOP <sup>e</sup>	molecular opacities [37]	EXO, DBW, STEL, E
SSHADE <sup>e</sup>	solid spectroscopy data [35]	E, C, EXO, ISM, PL
AMBDA <sup>d</sup>	collisions in plasmas (bibliography) ( <sup>a</sup> )	Nuclear Fusion
DESIRE <sup>d</sup>	radiative data for sixth row elements [3,38]	STEL, SOL, plasmas
DREAM <sup>d</sup>	radiative data for rare earths [39]	STEL, SOL, plasmas, lighting industry
IAMDB <sup>d</sup>	A+M spectroscopy, atomic collision ( <sup>a</sup> )	Astrophysics, other
PEARL <sup>d</sup>	atomic processes [40]	STEL, SOL, plasma, fusion
Clusters <sup>d</sup>	cluster size distributions, condensation ( <sup>a</sup> )	ISM, P, biology

<sup>a</sup> Paper in preparation <sup>b</sup> (FM, C) <sup>c</sup> (P, C) <sup>d</sup> (P, TC) <sup>e</sup> (FM, TC)

60 covering electron-impact ionisation and excitation cross sections, heavy-particle collision cross sections  
61 and plasma-wall interaction properties.

62 The first retrieval and display database system, the Atomic and Molecular Data Interactive System  
63 (AMDIS), was constructed in a mainframe computer for electron-impact ionisation and excitation cross  
64 sections of atoms and atomic ions in 1981 [43], with the database system being subsequently extended  
65 to include other collision processes. Currently the database system consists of eight sub-databases  
66 accessible via internet, full details are described by Murakami et al. [44].

67 Numerical data of collision cross sections and rate coefficients of various collision processes are  
68 compiled mainly from the published literature as well as bibliographic data and additional information  
69 such as experimental or theoretical methods used to derive the data are attached. Initially, data were  
70 collected for elements that were important mainly for fusion science; later the database was extended  
71 to include many more atoms and molecules applicable to various plasma applications.

72 Usually, several data sets obtained from different publications are stored for the same collision  
73 processes. Users can compare those data sets to check their reliability. Data can be queried by elements,  
74 charge states or various other query fields such as initial and final states, author, published year, and  
75 retrieved data are displayed as a numerical table or as a graph.

76 One of the sub-databases, AMDIS-IONIZATION has been available from the VAMDC portal with  
77 search functionality by element since 2017 [4]. AMDIS-IONIZATION has electron-impact ionisation  
78 cross sections and rate coefficients for atoms and atomic ions. Data sets of cross sections with collision  
79 energy or rate coefficients with electron temperature for single or multiple ionisation processes are  
80 available. Sometimes initial and final electronic states are available according to the original data  
81 source. In the future it is planned to add AMDIS-EXC (electron-impact excitation cross sections and  
82 rate coefficients for atoms and atomic ions) to the VAMDC portal.

### 83 2.1.2. VALD

84 The Vienna Atomic Line Database (VALD) compilation is a critically assessed collection of  
85 radiative transition data aimed primarily at the stellar astrophysics community. VALD contains data  
86 on energy levels, wavelengths, oscillator strengths and line broadening parameters for nearly all stable  
87 elements in the periodic table and for a few simple molecules. For atoms, VALD includes 6 ionisation  
88 stages. The VALD interface allows a search of the whole data collection or on a restricted subset that is  
89 based on high-precision laboratory measurements. The Moscow VAMDC node serves high-precision  
90 data only, while the Uppsala VAMDC node provides the most complete VALD data set.

91 VALD also includes atomic data for individual rare-earth elements/ions, also provided by the  
92 DREAM database<sup>7</sup> [45] (see Section 2.3.4). These atomic data are extracted via VALD extraction tools  
93 following an adopted quality ranking. Therefore, only a part of DREAM data collection is accessible  
94 through the VALD-VAMDC nodes.

95 VALD is under continuous development both in terms of functionality and data content. New  
96 data sets are systematically compared with existing ones and with experimental data in order to  
97 establish data quality ranking. For any given transition, all data elements are merged according to the  
98 ranking offering the best quality result for the end user while preserving all relevant bibliographic  
99 references. Recent developments include the gradual introduction of energy level and spectral line  
100 data for individual isotopes and isotopologues. Currently the work is complete for Li, Ca, Ti, Cu, Ga,  
101 Ba, Eu atoms and for isotopologues of CN, TiO, C<sub>2</sub>, CH, CO, OH, MgH and SiH. VALD now also  
102 provides data for the hyperfine-structure splitting of <sup>6</sup>Li I, <sup>7</sup>Li I, <sup>23</sup>Na I, <sup>27</sup>Al I, <sup>27</sup>Al II, <sup>39</sup>K I, <sup>40</sup>K I, <sup>41</sup>K I,  
103 <sup>45</sup>Sc I, <sup>45</sup>Sc II, <sup>47</sup>Ti I, <sup>49</sup>Ti I, <sup>47</sup>Ti II, <sup>49</sup>Ti II, <sup>50</sup>V I, <sup>51</sup>V I, <sup>51</sup>V II, <sup>55</sup>Mn I, <sup>55</sup>Mn II, <sup>57</sup>Fe I, <sup>59</sup>Co I, <sup>59</sup>Co II, <sup>61</sup>Ni I,  
104 <sup>63</sup>Cu I, <sup>65</sup>Cu I, <sup>67</sup>Zn I, <sup>67</sup>Zn I, <sup>69</sup>Ga I, <sup>69</sup>Ga I, <sup>71</sup>Ga I, <sup>71</sup>Ga II, <sup>85</sup>Rb I, <sup>87</sup>Rb I, <sup>87</sup>Sr II, <sup>89</sup>Y II, <sup>93</sup>Nb II, <sup>95</sup>Mo II,  
105 <sup>97</sup>Mo II, <sup>127</sup>I I, <sup>127</sup>I I, <sup>135</sup>Ba II, <sup>137</sup>Ba II, <sup>139</sup>La II, <sup>141</sup>Pr I, <sup>141</sup>Pr II, <sup>151</sup>Eu II, <sup>153</sup>Eu II, <sup>155</sup>Gd II, <sup>157</sup>Gd II, <sup>159</sup>Tb II,

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<sup>7</sup> <https://hosting.umons.ac.be/html/agif/databases/dream.html>

106  $^{165}\text{Ho I}$ ,  $^{165}\text{Ho II}$ ,  $^{171}\text{Yb II}$ ,  $^{173}\text{Yb II}$ ,  $^{175}\text{Lu I}$ ,  $^{175}\text{Lu II}$ ,  $^{176}\text{Lu I}$ ,  $^{181}\text{Ta I}$ ,  $^{181}\text{Ta II}$ ,  $^{191}\text{Ir I}$ ,  $^{193}\text{Ir I}$ ,  $^{203}\text{Tl I}$ ,  $^{205}\text{Tl I}$   
107 and  $^{209}\text{Bi III}$ . The latest developments of VALD and its interface to VAMDC have been presented in  
108 several refereed publications [46–49] and conference proceedings [50–52]. It should be noted that the  
109 VALD database is linked to the VAMDC Query Store (see Section 3.2.2).

### 110 2.1.3. NIST ASD

111 The Atomic Spectra Database (ASD) [7] at the National Institute of Standards and Technology  
112 (USA) contains critically evaluated atomic data including energy levels, radiative transition  
113 probabilities and oscillator strengths, ionisation potentials, and observed and accurately calculated  
114 wavelengths of spectral lines between the hard X-ray and infrared regions of spectra. As of July 2020,  
115 ASD provides data on more than 112,000 energy levels, 280,000 spectral lines and 118,000 radiative  
116 transition probabilities for elements from H ( $Z = 1$ ) to Ds ( $Z = 110$ ). The majority of the data on  
117 energies and spectral lines were collected and evaluated from experimental papers, and in most cases  
118 realistic uncertainties are provided as well. ASD is directly linked to the set of the NIST Atomic  
119 Spectroscopy Bibliographic Databases [53], which allows an immediate access to the original sources of  
120 data. In addition to a tabular output of data in various formats, ASD also offers rich graphical services,  
121 e.g. online-generated Grotrian diagrams of levels and transitions. ASD serves as the basis for the NIST  
122 LIBS (Laser-Induced Breakdown Spectroscopy) Database [54], which allows on-the-fly generation of  
123 realistic spectra for Saha–Boltzmann plasmas that are used for analysis of elemental abundances and  
124 diagnostics of terrestrial and astrophysical plasmas.

### 125 2.1.4. Spectr- $W^3$

126 The Spectr- $W^3$  project<sup>8</sup> is a long-term collaboration between the Russian Federal Nuclear Centre –  
127 All-Russian Institute of Technical Physics (RFNC-VNIITF) and the Joint Institute for High Temperatures  
128 of the Russian Academy of Sciences (JIHT RAS) [8]. At present, Spectr- $W^3$  is the largest available  
129 database providing information on spectral properties of multicharged ions. The database contains  
130 over 450,000 records of experimental, theoretical and compiled numerical data on ionisation potentials,  
131 energy levels, wavelengths, radiative and autoionisation widths, satellite-line intensity factors for free  
132 atoms and ions and also fitting parameters, and analytic formulae to represent electron-collisional cross  
133 sections and rates (optional). References to the original sources and comments on the methods of data  
134 acquisition, etc. are also provided. Since 2016, a new section of Spectr- $W^3$  providing graphical data on  
135 X-ray emission spectra (densitograms) recorded from various plasma sources has been made available  
136 to users. Densitogram graphic images are characterised with a set of fields enabling one to perform  
137 queries specifying the shortest and longest wavelengths of interest, the identification of up to five  
138 chemical elements and ionic isosequences, emission from which contributes to the recorded spectra,  
139 the upper and lower principal quantum numbers of optical single-electron transitions corresponding  
140 to the spectral lines pictured and the reference to the relevant publication. Densitogram database  
141 records are also supplied with comments elucidating details of the experimental measurements.

### 142 2.1.5. CHIANTI

143 CHIANTI<sup>9</sup>, first released in 1996 [55], is a well-established atomic database and modelling code  
144 for optically thin plasmas. For a recent overview of the status of the database and future plans, see [9].  
145 The database consists of a series of ASCII files with all the relevant atomic collisional and radiative  
146 rates (collisional excitation rates by electron and proton impact, transition probabilities, as well as  
147 theoretical/experimental wavelengths) required to calculate spectral line emissivities. The database

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<sup>8</sup> <http://spectr-w3.snz.ru>

<sup>9</sup> [www.chiantidatabase.org](http://www.chiantidatabase.org)

148 originally only included ions of astrophysical importance but in recent versions data for minor ions  
149 and some neutrals have also been added.

150 Radiative transition rates and wavelengths from CHIANTI versions 6 and 7.1 were included in  
151 VAMDC. The CHIANTI database also has ionisation/recombination rates and various other types  
152 of data that are specific for the modelling codes but these were not included in VAMDC. CHIANTI  
153 version 8 [56] included new atomic rates for ions in the Li, B and Ne isoelectronic sequences, plus  
154 atomic data for several iron ions participating in emission of light from the solar corona. Excitation  
155 rates among all states have been included (for modeling of high-density plasma), which has increased  
156 the size of the database significantly. Version 8 also changed the format of some of the main ASCII files.  
157 CHIANTI version 9 [57] then introduced a significant change in the structure of the data for several  
158 ions to allow the calculation of the emissivities of satellite lines, with autoionising states and rates  
159 having been added to those of the bound levels.

160 These changes mean that a straightforward update to include all the changes of CHIANTI version  
161 8 onwards within VAMDC could not be carried out, so at present the VAMDC portal only accesses  
162 CHIANTI version 7.1. CHIANTI version 10 is now in development and it is planned to integrate this  
163 version with the latest CHIANTI data into VAMDC.

#### 164 2.1.6. TIPbase-TOPbase

165 The Iron Project (IP) and The Opacity Project (OP) databases provide energy levels/terms,  
166 radiative transitions probabilities, photoionisation cross sections and collision strengths for a large  
167 selection of ions in the range H to Ni. The TOPbase contains the OP data for radiative processes  
168 [11,58,59], and the TIPbase the IP data for collisional and radiative processes [10]. The data have  
169 been calculated using state-of-the-art computer programs developed and maintained by the IP-OP  
170 members including the *R*-matrix suite of codes [60,61] and the AUTOSTRUCTURE code [62]. These  
171 data are relevant for experiment analysis, theoretical comparisons and for various astrophysical or  
172 laboratory experimental applications. The OP radiative data are used to calculate monochromatic and  
173 mean opacities [63] required in stellar codes and for the analysis of experiments. The TOPbase and  
174 TIPbase are hosted at the University of Strasbourg in France<sup>10</sup>. Sets of new (there were no data of  
175 that type in the database before) and recalculated data (with a better methodology) for existing data  
176 are being implemented in TOPbase for Fe I (new), Fe II (new) and Fe XVII (recalculated) as well as  
177 all the Ni ions (new); other recalculated ions will follow. A new service for opacity table is available  
178 on the TIPTOP webserver [64] (but not yet accessible through VAMDC). It should be noted that the  
179 TIPbase-TOPbase databases are linked to the VAMDC Query Store (see Section 3.2.2).

#### 180 2.1.7. Stark-B

181 Stark-B [12,65–67] is devoted to the modelling and spectroscopic diagnostics of various plasmas  
182 in astrophysics, laboratory experiments, laser equipment design, laser produced plasma analysis  
183 and inertial fusion research. It contains Stark widths and shifts of isolated lines of atoms and ions  
184 due to collisions with electrons, protons, ionised helium (the most important colliders for stellar  
185 atmospheres) and other ions. The data are calculated using the semi-classical perturbation [68] and  
186 modified semi-empirical methods [69]. Stark-B is continuously updated by adding new data and  
187 by introducing new facilities for their use. Under the website option “Data history” there are “New  
188 datasets” and “Updated datasets”, which make available a description of newly added data including  
189 the date of import and details of the modifications for revised data. In order to enable inclusion of  
190 data from Stark-B in the computer codes used for stellar atmospheres modelling and other numerical  
191 calculations, it is possible to fit tabulated data with temperature. In particular, a fitting formula for  
192 interpolation of the displayed data for different temperatures has been derived [70]. Thus, to each

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<sup>10</sup> <http://cdsweb.u-strasbg.fr/OP.htx>

193 table of Stark widths and shifts, an additional table has been added with the coefficients needed for the  
194 fitting formula. The latest updates are further described in the current issue [13]. It should be noted  
195 that the Stark-B database is linked to the VAMDC Query Store (see Section 3.2.2).

#### 196 2.1.8. CDMS and JPL Spectral Line Catalog

197 Both these databases<sup>11</sup> provide spectral data for molecular species, which are or may be observed  
198 in various astronomical sources (usually) by radio astronomical means or for use in remote sensing.  
199 The JPL catalog [15,71,72] and the CDMS [14,72–74] have been previously described to some extent in  
200 the literature. Briefly, the database content is generally restricted to effective Hamiltonian predictions  
201 and associated assigned experimental data for quantum transitions with entry fields including line  
202 position with accuracy, intensity, lower state energy and quantum numbers. These restrictions facilitate  
203 transfer of high-precision laboratory data into comprehensive predictions within the associated range  
204 of quantum numbers, and reconciliation and/or extension of models from multiple laboratory studies.  
205 Separate entries exist for different isotopic species and usually also for different vibrational states.  
206 Updates and new entries to the spectral data are performed aperiodically, with focus on detection in  
207 the interstellar medium as well as candidates for terrestrial remote sensing target molecules.

208 The incorporation of these two databases in VAMDC, and thus the application of its standards  
209 (see Section 3.1.1), not only greatly simplified the interoperability between the databases and improved  
210 the readability of the content (e.g. quantum number format), but also provided additional features and  
211 information. A listing of energy levels as well as all files that have been used to generate the data are  
212 commonly provided. Partition functions are now tabulated for 110 temperatures up to 1000 K. In the  
213 context of VAMDC, a Python library (`vamdc1ib`) has been developed that allows queries of data via  
214 VAMDC protocols with the information being stored in a local `SQLITE3` database for use in third-party  
215 applications (e.g. `XCLASS`, see below in the section of use cases). Both databases are linked to the  
216 VAMDC Query Store (Section 3.2.2), and thus support VAMDC's generation of digital object identifiers  
217 (DOIs) for individual queries that can be used to cite this data in publications.

218 Creating new entries or updating existing ones is an important part of the work for the CDMS. As  
219 of July 2020, there are 1020 entries in the CDMS, up from 808 four years ago. Recent activities have  
220 emphasised species that are or may be observable with the Atacama Large Millimeter/submillimeter  
221 Array (ALMA), the Northern Extended Millimeter Array (NOEMA) and similar facilities. Examples  
222 include metal-containing di- and triatomics, which are relevant for the circumstellar envelopes of  
223 late-type stars, small to moderately sized organics, including cyclic molecules, which were or may be  
224 detected in star-forming regions, and several radicals or cations. Some effort has been made to make  
225 vibrationally excited state data available since transitions pertaining to low-lying excited vibrational  
226 states have been observed for several small to mid-sized organics (< 15 atoms) in the dense and warm  
227 parts of star-forming regions. Very highly excited states of diatomics and some larger molecules, such  
228 as HCN, have been detected in particular in the envelopes of C- and O-rich late-type stars. A detailed  
229 account of these activities is planned in the near future.

#### 230 2.1.9. HITRAN

231 The HITRAN molecular spectroscopic database [16] is a canonical compilation of molecular  
232 spectroscopic parameters that are required for the input into the radiative-transfer codes. HITRAN  
233 provides the best unique parameter values assimilated from both experimental and theoretical  
234 studies. Before adapting data to the database, the HITRAN group performs independent evaluations  
235 (controlled laboratory, atmospheric retrievals and theoretical analyses) wherever possible. While  
236 the target audience of HITRAN are scientists that study terrestrial and planetary atmospheres, the  
237 applications of HITRAN span a great many fields of science, engineering and medicine. The database

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<sup>11</sup> <https://cdms.astro.uni-koeln.de>, <https://spec.jpl.nasa.gov>

238 was first established several decades ago [75] and has been under continuous development since  
239 then [16,76–83]. The latest edition of the database is HITRAN2016 [16] and is distributed through  
240 HITRAN*Online* [84] that is accessible through the VAMDC portal. The VAMDC portal provides access  
241 to a traditional line-by-line high-resolution section of HITRAN, which contains spectral parameters  
242 for 49 molecules along with their significant isotopologues appropriate for terrestrial and planetary  
243 atmospheric applications. HITRAN provides references to the original sources for the majority of the  
244 parameters for every transition. The details of how such referencing was incorporated is described  
245 by Skinner et al. [85] in this special issue. It is worth pointing out that with an exception of some  
246 diatomic molecules (including hydrogen halides) for which the line lists can be used at temperatures  
247 up to 5000 K or higher, the majority of the HITRAN line lists are intended to be used at the lower  
248 temperatures encountered in the terrestrial atmosphere.

249 For higher temperature applications, it is recommended to use the HITEMP database [86], which  
250 mimics the format of HITRAN but contains a substantially larger amount of lines. However, at the  
251 present time, the HITEMP database provides data for only eight molecules [86–89], and is not currently  
252 accessible through VAMDC due to the large number of transitions it contains.

253 HITRAN also provides a section that contains high-resolution experimental cross sections for  
254 molecules with very dense spectra that are not amenable to a full quantum-mechanical description. A  
255 recent update [90] provided spectra of almost 300 molecules at various pressures and temperatures.  
256 There is also a section of the compilation that provides collision-induced absorption cross sections,  
257 which has been updated recently [91]. These data are not accessible through VAMDC yet but can  
258 be accessed through HITRAN*Online*<sup>12</sup> or through the HITRAN Application Programming Interface  
259 (HAPI) [92]. A very extensive effort is currently underway to release the new HITRAN2020 edition of  
260 the database.

#### 261 2.1.10. S&MPO

262 S&MPO (Spectroscopy and Molecular Properties of Ozone) is an information system [17] jointly  
263 developed by Reims University (France), Institute of Atmospheric Optics (Russia) and Tomsk State  
264 University (Russia). The line-by-line list of vibration-rotation transitions, energy levels, transition  
265 moments and other related information can be requested from S&MPO via the VAMDC portal.  
266 Since the previous edition of VAMDC [3], considerable new spectroscopic information has been  
267 included using experimental data and extended analysis of ozone bands in the infrared [93] and  
268 isotopic spectra enriched by <sup>17</sup>O and <sup>18</sup>O oxygen [94,95]. Supplementary information concerning  
269 theoretical spectra simulation, comparisons with experimental records, dipole moment functions [96]  
270 and *ab initio* intensities for strong lines [97] can be accessed via the Reims<sup>13</sup> and Tomsk<sup>14</sup> sites. The  
271 S&MPO interactive software was completely rewritten to make it relevant to current trends in internet  
272 application development. A new version 3.0 of the S&MPO relational database and information  
273 system is now operational and provides supplementary functionalities for the fully updated graphical  
274 interface. More information about the version 3.0 S&MPO information system can be found on its  
275 public website<sup>15</sup>. Applications of the S&MPO may include education/training in molecular and  
276 atmospheric physics, studies of radiative processes and spectroscopic analysis.

#### 277 2.1.11. MeCaSDa, ECaSDa, TFMecaSDa, SHeCaSDa, GeCaSDa, RuCaSDa, TFSiCaSDa, UHeCaSDa

278 These databases contain calculated rovibrational transitions (mostly infrared absorption and  
279 also some Raman scattering lines) for highly symmetrical molecules. They result from the analysis

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12 <https://hitran.org>

13 <http://smpo.univ-reims.fr>

14 <http://smpo.iao.ru>

15 [https://smpo.univ-reims.fr/news/en\\_2019-09-25\\_02-22-19](https://smpo.univ-reims.fr/news/en_2019-09-25_02-22-19)

280 and fit of effective Hamiltonian and transition moments using experimental spectra recorded at high  
281 resolution. The calculation uses a model [98] and programs [99] developed by the group at the  
282 Laboratoire Interdisciplinaire Carnot de Bourgogne, Dijon, France, and based on group theory and  
283 tensorial formalism [100].

284 The MeCaSDa database [101] contains methane ( $\text{CH}_4$ ) lines, which constitutes the main research  
285 subject of the Dijon group. It is Dijon's biggest database and is of importance for atmospheric and  
286 planetary applications. Its contents have recently been updated, and it now has more than 16 million  
287 lines [18].

288 Other databases for several molecules of either atmospheric, planetological or industrial  
289 applications have been significantly updated recently [18]: ECaSDa ( $\text{C}_2\text{H}_4$  found in Earth's and  
290 planetary atmospheres [101]), TFMeCaSDa ( $\text{CF}_4$  found in Earth's atmosphere), SHeCaSDa ( $\text{SF}_6$  found  
291 in Earth's atmosphere), GeCaSDa ( $\text{GeD}_4$  found in giant planets' atmospheres) and RuCaSDa ( $\text{RuO}_4$   
292 important for the nuclear industry).

293 Two new databases have been added recently: TFSiCaSDa [19] concerning the  $\text{SiF}_4$  molecule with  
294 applications to volcanic gases and UHeCaSDa ( $\text{UF}_6$ ) for applications for the nuclear industry. This  
295 latter database is an exception: no experimental data are publicly available for this peculiar radioactive  
296 molecule and calculations are only based on literature data [102,103]. More databases of such highly  
297 symmetrical molecules maybe developed in the near future. The databases SHeCaSDa, MeCaSDa,  
298 GeCaSDa, TFMeCaSDa and RuCaSDa are linked with the Query Store service (Section 3.2.2), while the  
299 databases ECaSDa, TFSiCaSDa and UHeCaSDa are currently being connected to the Query Store.

#### 300 2.1.12. CDS-296, CDS-1000, CDS-4000, ASD-1000, NOSD-1000 and NDS-1000

301 Six molecular databanks in VAMDC of atmospheric and astrophysical interest have been provided  
302 by the Laboratory of Theoretical Spectroscopy, V.E. Zuev Institute of Atmospheric Optics, Siberian  
303 Branch, Russian Academy of Sciences, Russia. These include three versions of the Carbon Dioxide  
304 Spectroscopic Databank (CDS-296, CDS-1000, CDS-4000), the Acetylene Spectroscopic Databank  
305 (ASD-1000), the Nitrous Oxide Spectroscopic Databank (NOSD-1000) and the Nitrogen Dioxide  
306 Spectroscopic Databank (NDS-1000). These databanks provide positions, intensities, air- and  
307 self-broadened half-widths, coefficients of temperature dependence of the half-widths and quantum  
308 numbers associated with the transitions. The line positions and intensities are calculated within the  
309 framework of the method of effective operators. The line shape parameters are calculated using  
310 different theoretical approaches or empirical equations in terms of the rotational quantum numbers.

311 CDS-296 and CDS-1000 have been described in our previous paper [3]. CDS-296 has been  
312 updated recently [20] to improve the line parameters accuracy. CDS-4000 contains more than 628  
313 million lines of the four most abundant isotopologues of carbon dioxide and covers the 226–8310  
314  $\text{cm}^{-1}$  wavenumber range [21]. The reference temperature is  $T_{\text{ref}} = 296$  K and the intensity cutoff  
315 is  $10^{-27} \text{ cm}^{-1}/(\text{molecule cm}^{-2})$  at 4000 K. ASD-1000 has more than 30 million lines of the principal  
316 isotopologue of acetylene in the 3–10000  $\text{cm}^{-1}$  spectral range [24]. The database is adopted for the  
317 temperatures up to 1000 K with an intensity cutoff  $10^{-27} \text{ cm}^{-1}/(\text{molecule cm}^{-2})$ . The line intensities  
318 and pressure broadening coefficients are given for  $T_{\text{ref}} = 296$  K. NOSD-1000 contains more than 1.4  
319 million lines of the principal isotopologue of nitrous oxide and covers the 260–8310  $\text{cm}^{-1}$  region [22].  
320 The intensity cutoff is at  $10^{-25} \text{ cm}^{-1}/(\text{molecule cm}^{-2})$  at  $T_{\text{ref}} = 1000$  K. Finally, the NDS-1000 has  
321 more than 1 million lines in the 466–4776  $\text{cm}^{-1}$  wavenumber range [23]. The intensity cutoff is at  
322  $10^{-25} \text{ cm}^{-1}/(\text{molecule cm}^{-2})$  at  $T_{\text{ref}} = 1000$  K. The broadening parameters are given for two reference  
323 temperatures:  $T_{\text{ref}} = 296$  K and  $T_{\text{ref}} = 1000$  K.

324 Currently, the above mentioned databanks are presented in VAMDC as separate nodes with a  
325 similar basic set of "restrictables"<sup>16</sup> parameters (wavenumber, wavelength, line strength, InChIKey

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<sup>16</sup> Restrictables refer to the type of data queried by VAMDC (<https://standards.vamdc.eu/dictionary/restrictables.html>).

326 and state energies). The common set of returnable entities includes radiative transitions, sources,  
327 isotopic species, environment signatures and function descriptions for the temperature and pressure  
328 dependencies of line shape parameters. The parametric content of these returnables however, depends  
329 on the original structure of the particular databank. Unification of these databanks, which is a step  
330 necessary for their merging into a single VAMDC node, is subject of future work.

331 Besides being available through VAMDC, the databanks can be downloaded from the IAO ftp  
332 server<sup>17</sup> where they are presented in the original tabular format.

#### 333 2.1.13. SESAM

334 SESAM<sup>18</sup> is restricted to the electronic spectra of molecular hydrogen and its deuterated  
335 substitutes, as well as CO. The hydrogen spectra includes the Lyman and Werner band systems as well  
336 as B'-X, D-X electronic bands. The SESAM database allows queries, within a specific wavelength range,  
337 of the properties of available transitions of a selected molecule. The transitions are in the Vacuum  
338 Ultra Violet (VUV) range. It is also possible to download the full range of data for a particular goal.  
339 Different additions are considered, e.g. the query of these molecular transitions at any redshift, which  
340 can be interesting for extragalactic observations where the spectrum is shifted in the visible. Since 2016  
341 the CO molecule has been added. Further information and the latest updates are described in this  
342 Special Issue [13]. It should be noted that the SESAM database is linked to the VAMDC Query Store  
343 (Section 3.2.2).

#### 344 2.1.14. W@DIS

345 The W@DIS databases are part of the information system [25] designed to provide access to  
346 both tabular and graphical data, as well as information [104]<sup>19</sup> and ontologies [105] for quantitative  
347 molecular spectroscopy necessary for solving fundamental and applied problems in a number of subject  
348 areas: atmospheric spectroscopy of planets and exoplanets, astronomy, etc. The semantic information  
349 system W@DIS is the next-generation molecular spectroscopy information system, based on application  
350 of Semantic Web technologies to its tabular and graphical information resources [106,107]. The W@DIS  
351 information system is available and hosted at the V.E. Zuev Institute of Atmospheric Optics in Tomsk,  
352 Russia<sup>20</sup>. This system can be a prototype for semantic information systems in the atomic, ionic  
353 and solid-state spectroscopy to be used by the VAMDC consortium. Meanwhile some data such as  
354 transitions are accessible from the VAMDC portal; they can be displayed via the "Molecular XSAMS to  
355 HTML" visualisation tool.

#### 356 2.1.15. KIDA

357 The KInetic Database for Astrochemistry (KIDA<sup>21</sup>) [26,27] is a compilation of kinetic data  
358 (chemical reactions and associated rate coefficients) used to model chemistry in astrophysical  
359 environments (interstellar medium, protoplanetary disks, planetary atmospheres, etc.). In addition  
360 to detailed information on each reaction (e.g. temperature range of validity of the rate coefficients,  
361 reference and uncertainty), particular attention is given to the quality of the data, which is evaluated  
362 by a group of experts in the field. Since 2016, KIDA also compiles data used to compute chemical  
363 reactions occurring on the surface of interstellar dust grains (branching ratios, activation energies  
364 and barrier width) and desorption/diffusion of species on these surfaces (desorption and diffusion  
365 energies).

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17 <ftp://ftp.iao.ru/pub/>

18 <http://sesam.obspm.fr/>

19 "information" is interpreted in accordance with the same term defined in the given reference

20 <http://wadis.saga.iao.ru>

21 <http://kida.astrophy.u-bordeaux.fr>

#### 366 2.1.16. UDfA

367 The UMIST Database for Astrochemistry (UDfA), first released to the public in 1991 [108], contains  
368 basic chemical kinetic data and associated software codes and documentation for modelling the  
369 chemical evolution of interstellar clouds and the circumstellar envelopes of evolved AGB stars. The  
370 core of the data, which can be accessed via its website<sup>22</sup> in addition to VAMDC, consists of reaction  
371 rate coefficients of several thousand gas-phase reactions and is supplemented by more restricted  
372 data sets concerning the chemistry of deuterium fractionation. The database does not contain any  
373 surface chemistry but a file of surface binding energies, which allows processes such as reaction and  
374 desorption to be taken into account, is supplied. Where possible, and in line with VAMDC policy,  
375 a great deal of effort has been made to identify the precise source of each datum entry through the  
376 application of its DOI, in particular for those rate coefficients measured experimentally. Software codes  
377 for calculating the chemical evolution of interstellar and circumstellar regions are also provided as  
378 are codes that generate UDfA output files in the form needed for radiative transfer codes such as  
379 RADEX<sup>23</sup>, RATRAN<sup>24</sup> and RADMC-3D<sup>25</sup> used to calculate emergent molecular line profiles from  
380 these regions. A major revision of the 2013 release [28], including the review of current data and the  
381 identification of new reactions, particularly those associated with chlorine chemistry and with the  
382 formation of metal oxides, hydroxides and chlorides in oxygen-rich AGB stars, is underway with a  
383 public release due by the end of 2020.

#### 384 2.1.17. BASECOL

385 The BASECOL database collects, from the refereed literature, the rate coefficients for the excitation  
386 of rotational, vibrational and rovibrational levels of molecules by atoms, molecules and electrons. The  
387 processes are described in the temperature ranges relevant to the interstellar medium, to circumstellar  
388 atmospheres and to cometary atmospheres. The BASECOL database is currently the sole VAMDC  
389 connected database that implements the Java version of the node software<sup>26</sup>. It can be displayed  
390 from the VAMDC portal with the "Collisional data XSAMS to HTML" processor and is accessible  
391 from the SPECTCOL tool [109,110]. Since its last review paper in 2013 [29] the scientific content of  
392 the database is updated with published data. Since the last VAMDC review paper in 2016 [3], the  
393 technical components of the database have been entirely replaced [30] with the internal structure of  
394 the database, and the data ingestion files have been made compliant with the metadata necessary for  
395 VAMDC interoperability. The public graphical interface has been changed to a simpler system. The  
396 connection of BASECOL with the Query Store (Section 3.2.2) is in a final testing phase. A complete  
397 description of the new BASECOL technical design and updates can be found in this Special Issue [30].

#### 398 2.1.18. MOID

399 The MoID VAMDC node [31,32] provides data for plasma modelling, e.g. for modelling different  
400 stellar atmospheres, early Universe chemistry and analysis of the kinetics of laboratory plasma. MoID  
401 contains photodissociation cross sections for individual rovibrational states of diatomic molecular ions  
402 as well as corresponding data on molecular species and molecular state characterisations calculated  
403 using a quantum mechanical method described in [111]. Since the previous VAMDC review [3] large  
404 amounts of new data concerning alkali molecular ions have been included from reference [112].

405 The node is hosted at the Belgrade Astronomical Observatory<sup>27</sup>. It has enabled fairly easy access  
406 to data (in tabulated and graphical form) of thermally averaged photodissociation cross sections

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22 <http://www.udfa.net>

23 <https://personal.sron.nl/~vdtak/radex/index.shtml>

24 <https://personal.sron.nl/~vdtak/ratran/frames.html>

25 [www.ita.uni-heidelberg.de/~dullemond/software/radmc-3d/](http://www.ita.uni-heidelberg.de/~dullemond/software/radmc-3d/)

26 [www.vamdc.org/activities/research/software/java-nodesoftware/](http://www.vamdc.org/activities/research/software/java-nodesoftware/)

27 <http://servo.aob.rs/mold>

407 across the available spectrum at a requested temperature in order to facilitate atmospheric modelling  
408 and other numerical calculations [113]. Future plans are to include new (i.e. complex) molecules of  
409 astrophysical importance. The MolD database is linked to the Query Store service (Section 3.2.2).

#### 410 2.1.19. BeamDB

411 BeamDB (the Belgrade electron-atom/molecule DataBase) is a collisional database, in which  
412 electrons are projectiles while targets are considered to be atoms and molecules [33]. Interactions  
413 of electrons with atoms and molecules are presented as both differential and integral cross sections  
414 for processes such as elastic scattering, excitation and ionisation [114]. Since the previous review of  
415 VAMDC [3] a considerable volume of new collisional data on metal atom targets have been included  
416 from the published sources (e.g. for bismuth [115] or zinc [116]) and selected molecules (e.g. for  
417 methane [113] or nitrous oxide [32]). Curation and maintenance of electron collisional data is relevant  
418 in many research areas such as astrophysics [117], plasma [118], radiation damage [119] or in lighting  
419 applications [120]. The plan for the future expansion of the database is to include ions as new  
420 targets [121]. BeamDB<sup>28</sup> is hosted at the Belgrade Astronomical Observatory and is linked to the Query  
421 Store service (Section 3.2.2).

#### 422 2.1.20. IDEADB

423 The Innsbruck Dissociative Electron Attachment (DEA) database node collects relative partial  
424 cross sections for dissociative electron attachment processes of the form:  $AB + e^- \rightarrow A^- + B$ , where AB  
425 is a molecule. Queried identifiers are searched in both products and reactants of the processes. XSAMS  
426 files (see Section 3.1.1) are then returned which describe the processes found including numeric values  
427 for the relative partial cross sections of the dissociative electron attachment reactions. Additionally, a  
428 visual representation of the cross sections can be viewed on the web site. Since 2016 the possibility to  
429 add cross sections for cationic products and resolution of several minor issues have been addressed. It  
430 is planned to modify the database structure, so that measurements in matrices such as water or helium  
431 nanodroplets can be added. The node<sup>29</sup> is hosted and maintained by the group of Paul Scheier at the  
432 University of Innsbruck, Austria.

#### 433 2.2. VAMDC Data Nodes that Have not Evolved since 2016

434 There have been no changes to some databases and nodes since 2016. These will be described in  
435 this section, and more information can be found in our previous publication [3]. It should be noted that  
436 these databases contain quite unusual species and processes for the VAMDC e-infrastructure, for which  
437 the current VAMDC visualisation tools and even the current VAMDC standards lack features that  
438 would allow a full display of the databases contents. Therefore at present VAMDC mainly provides  
439 only a simple view of those databases.

#### 440 2.2.1. LASp

441 The LASp (Laboratorio di Astrofisica Sperimentale) database is hosted at the Catania  
442 Astrophysical Observatory in Italy<sup>30</sup> and additional information can be found at its URL<sup>31</sup>. LASp  
443 spectra are taken by using *in situ* techniques and equipment especially developed to analyse the effects  
444 of irradiation (ion and/or UV photons) and thermal cycling (down to 10 K) by infrared, Raman and  
445 UV-VIS-NIR spectroscopy. Analysed materials include frozen gases, solids samples and meteorites.

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28 <http://servo.aob.rs/emol>

29 <https://ideadb.uibk.ac.at/>

30 <http://vamdcclasp.oact.inaf.it/GUI/index>

31 <http://www.oact.inaf.it/weboac/labsp/index.html>

446 The main application field up until now has been in astrophysics, and over the years many hundreds  
447 of ice mixtures of various compositions and of solids have been studied.

448 Through the VAMDC portal, transmission and optical depth data for water-ice experiments are  
449 available [122,123]. The public database also includes optical constants of solid-state CO, CO<sub>2</sub> and  
450 CH<sub>4</sub> deposited at various temperatures.

### 451 2.2.2. PAH

452 The Cagliari–Toulouse PAH theoretical spectral database [36] is a joint effort by the groups of  
453 G. Mulas (INAF-OAC) and C. Joblin (Univ. Toulouse III/CNRS-IRAP) aimed at providing all the  
454 "ingredients" needed for modelling the photophysics of individual polycyclic aromatic hydrocarbons  
455 (PAHs) in space, mainly in photon-dominated interstellar and circumstellar environments. It includes  
456 basic structural properties of PAHs in four charge states (-1, 0, +1 and +2), ionisation potentials and  
457 electron affinities, harmonic vibrational analyses and vertical photoabsorption electronic spectra. The  
458 link to the "old" database with flat files, which includes more data than available through VAMDC, is  
459 still online<sup>32</sup>. The web interface to the relational database, holding the data available through VAMDC,  
460 is hosted at the Cagliari Observatory in Italy<sup>33</sup>. An effort is underway to develop import tools that will  
461 feed the relational database, and we expect some substantial changes within a year's time. Currently,  
462 from the VAMDC portal it is possible to obtain molecular structures, corresponding energies and  
463 vibrational analyses for a number of PAHs in different ionisation states. The electronic photoabsorption  
464 spectra are not available yet through VAMDC but will be in the near future.

### 465 2.3. Databases in the Process of Being Connected to VAMDC

#### 466 2.3.1. ExoMolOP

467 The ExoMol project provides molecular line lists for exoplanet and other atmospheres [124] with  
468 a particular emphasis on studies of hot atmospheres. Besides line lists, which are stored as states  
469 and transitions files [125], the ExoMol database<sup>34</sup> stores a variety of other associated data including  
470 partition functions, state lifetimes, cooling functions, Landé g-factors, temperature-dependent cross  
471 sections, opacities, pressure broadening parameters, *k*-coefficients and transition dipoles. These data  
472 and the associated data structure are described in the database release papers [126,127]. The line  
473 lists provided by ExoMol are huge and are too big to be handled by the VAMDC portal; this issue is  
474 described below.

475 Recently a new offshoot of the ExoMol project called ExoMolOP has been created, which contains  
476 opacity cross sections and *k*-tables [128] for molecules of astrophysical interest [37]. This database  
477 is built on ExoMol data but contains input from HITRAN [16], the empirical MolList database of  
478 Bernath [129] and NIST for selected atoms. ExoMolOP provides data on a grid of 22 pressures and 27  
479 temperatures on a grid of wavelengths for each species. By comparison with the unprocessed ExoMol  
480 data, these provide a comparatively compact representation of the absorption property of each species.  
481 An implementation of the ExoMolOP data within the VAMDC portal is currently in progress.

#### 482 2.3.2. SSHADE in VAMDC

483 Currently VAMDC allows access to the original GhoSST database<sup>35</sup>(Grenoble astrophysics  
484 and planetology Solid Spectroscopy and Thermodynamics) to search for a few pure and mixed  
485 molecular solids through their constituent species and to retrieve their infrared spectra, either as

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32 <https://astrochemistry.oa-cagliari.inaf.it/database/>

33 <https://qchitool-pah-dev.oa-cagliari.inaf.it/>

34 <http://www.exomol.com>

35 <https://ghosst.osug.fr/>

486 absorption coefficients or as optical constants. SSHADE<sup>36</sup> [35] is a database infrastructure of solid-state  
487 spectroscopy that hosts spectral data of many different types of solids including ices, snows, minerals,  
488 carbonaceous matters, meteorites, interplanetary dust particles and other cosmo-materials covering  
489 a wide range of wavelengths: from X-rays to millimeter wavelengths. The data are collected from a  
490 consortium of partners<sup>37</sup>, which provide their data in their own database of the SSHADE infrastructure.  
491 Currently a “band list” database of molecular solids is under development in the frame of the  
492 Europlanet-2024 research infrastructure program. It will host critical compilations of the position,  
493 intensity, width and vibration modes of absorption bands (visible-infrared or Raman active) of pure  
494 and mixed molecular solids as well as for several types of molecular compounds such as hydrates  
495 and clathrate hydrates. Both the SSHADE spectral databases and the band list database will be linked  
496 to VAMDC, but this will require an upgrade of the XSAMS data model (see Section 3.1.1) in order to  
497 describe the fundamental solid constituents better. With such databases, VAMDC will allow the user  
498 to retrieve and compare the band parameters of molecular species in both gaseous and solid states,  
499 and therefore, will allow them to determine which one does actually contribute to observed absorption  
500 features. This capability is particularly useful in environments where both phases coexist, such as  
501 planetary atmospheres with aerosols.

### 502 2.3.3. AMBDAS

503 AMBDAS (Atomic and Molecular Bibliographic Data System)<sup>38</sup> is a library of around 50,000  
504 references to publications in the scientific literature concerning collisional and plasma-material  
505 interactions of relevance to nuclear fusion energy research. An online, browser-based searchable  
506 interface allows the database to be queried by reactant species, charge state and process type as well as  
507 by author, journal and title keyword.

508 Integration of AMBDAS within the VAMDC infrastructure is planned for release in 2020 as part  
509 of an upgrade to the database software, which includes a recently developed DOI-centred reference  
510 management library [85] and an updated classification of plasma processes [130]. In addition to a new  
511 search interface, VSS2 queries and XSAMS output (see Section 3.1.1) are supported. The AMBDAS  
512 system will be queried by species and processes, and so will be accessible from the species database.  
513 In addition, since the AMBDAS system is a bibliographic database, it will be queried through the new  
514 bibliographic service described in Section 6.5.

### 515 2.3.4. DREAM-DESIRE

516 The Database of Rare Earths At Mons University (DREAM) contains information concerning  
517 the radiative parameters (wavelengths, transition probabilities and oscillator strengths) for more than  
518 72,000 spectral lines belonging to the lower ionisation stages of lanthanide elements ( $Z = 57$  to  $71$ ),  
519 from neutral to triply ionised species. This database, originally created by Biémont et al. [131] and  
520 recently updated by Quinet and Palmeri [39], is hosted by Mons University<sup>39</sup>. All the data tabulated in  
521 DREAM have been determined from detailed pseudo-relativistic Hartree-Fock calculations including  
522 core-polarisation effects [132,133] carried out by the Atomic Physics and Astrophysics group at Mons  
523 University, Belgium. The accuracy of the theoretical results have been assessed through comparisons  
524 with experimentally measured radiative lifetimes using laser-induced fluorescence spectroscopy. The  
525 Database on Sixth Row Elements (DESIRE) contains the same type of information as DREAM, but is  
526 dedicated to the elements of the sixth row elements of the periodic table ( $Z = 72$  to  $86$ ). This database<sup>40</sup>  
527 is described in [38].

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36 <http://www.sshade.eu>

37 <https://wiki.sshade.eu/ssshade/databases>

38 <https://amdis.iaea.org/databases/>

39 <http://hosting.umons.ac.be/html/agif/databases/dream.html>

40 <http://hosting.umons.ac.be/html/agif/databases/desire.html>

### 528 2.3.5. IAMDB

529 The volume of high-precision data generated by the Indian atomic and molecular community is  
530 quite substantial. This is evident from the number of articles published by various groups. However,  
531 such data are not well organised and, hence, very difficult to retrieve for further use. This is the reason  
532 for the requirement of an atomic and molecular data repository in India, which has been envisaged for  
533 many years now. The Indian Atomic and Molecular DataBase (IAMDB<sup>41</sup>) is the outcome of such an  
534 effort. With the help of the VAMDC interface, the data generated and gathered in IAMDB can be easily  
535 retrieved by any user.

536 In the last few years a great deal of electron scattering data has been produced in India. In  
537 particular, partial and total electron ionisation cross sections have been measured over an extended  
538 energy regime for about two dozen organic molecules important to radiation biology [134,135]. Since  
539 many of these systems are in solid form at room temperature, a new experimental technique was  
540 employed for the measurements. The result of some important ones like DNA and RNA bases are  
541 reported in [134,135]. The same group has also measured dissociative electron attachment cross  
542 sections for several organic molecules [136]. On the other hand, Antony and coworkers have produced  
543 a large quantity of electron scattering data, in particular for those molecules and radicals which are  
544 difficult to measure [137,138]. Recent calculations from this group include positron scattering from a  
545 variety of atoms and molecules [139,140] and photoionisation cross sections for polyatomic molecules  
546 [141,142]. Once these electron/positron/photon collision data are incorporated into IAMDB, it will be  
547 integrated with VAMDC.

### 548 2.3.6. PEARL

549 The PEARL (Photonic Electronic Atomic Reaction Laboratory) database in the Korea Atomic  
550 Energy Research Institute (KAERI) includes electron impact ionisation (EII), recombination and  
551 photoionisation for atoms and ions. The EII [143] and the dielectronic recombination (DR) [144] have  
552 been calculated using a relativistic distorted wave approximation, and the photoionisation [145] has  
553 been calculated using a non-iterative eigenchannel *R*-matrix method for the ground and lower excited  
554 levels of atomic ions below  $Z = 30$ , which are of interest in astrophysics. The EII [146] and the DR [147]  
555 calculations have also been performed for tungsten (*W*,  $Z = 74$ ) ions, which are essential in fusion  
556 tokamak research. The calculated cross section data can be graphically displayed on the PEARL web  
557 site<sup>42</sup>, together with other available experimental and theoretical data for comparison, the numerical  
558 data can be also downloaded. Recently a collisional-radiative model (CRM) for low-temperature  
559 plasma has been developed and the electron impact excitation (EIE) data for the levels considered in  
560 the model have been calculated and compiled. The calculated line ratios of He I can be displayed as a  
561 function of the electron temperature and density on the website. CRM results for Ar I [148] will be  
562 uploaded in the near future.

### 563 2.3.7. Clusters

564 Clusters are complexes of two up to several million atoms and/or molecules which bridge the  
565 gap between molecular physics and solid-state physics. The addition or removal of a single atom  
566 or molecule from a cluster may dramatically change its properties. Interesting attributes in cluster  
567 physics are e.g. cluster structures, bond lengths and bond dissociation energies. These properties can  
568 be extracted by combining experimental techniques such as mass spectrometry and/or spectroscopy  
569 in combination with quantum chemical simulations.

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<sup>41</sup> [www.iamdb.org.in](http://www.iamdb.org.in)

<sup>42</sup> <http://pearl.kaeri.re.kr>

570 Clusters are not yet addressed by VAMDC. Inclusion of clusters in VAMDC requires the addition  
571 of a section to the schema of VAMDC to describe the cluster data. We propose to develop a two-layer  
572 implementation of the node. The first layer – which will be available in the portal as well – is for  
573 selecting the dominant species of interest (for example “(CO<sub>2</sub>)(H<sub>2</sub>O)”). This will return all datasets  
574 with clusters of “(CO<sub>2</sub>)<sub>n</sub>(H<sub>2</sub>O)<sub>m</sub>”, ( $m, n > 0$ ). Often, the produced mass spectra display features of  
575 many different cluster ions, because impurities are attached to the clusters of interest. Fragmentation  
576 of larger molecules may also display features of further non-stoichiometric cluster progressions. Thus,  
577 different queries return the same dataset. On the website of the node itself we will offer more filter  
578 options:

- 579 • Method of cluster formation (supersonic expansion, seeded beam, gas aggregation, electrospray  
580 ionization, helium nanodroplets, ...)
- 581 • Method of ionization (electrospray ionization, matrix-assisted laser desorption/ionization,  
582 electron impact, photo ionization, ...)
- 583 • Steps in between (tandem mass spectrometry, collision-induced dissociation, ...)
- 584 • Analysis method (time-of-flight, quadrupole, ion cyclotron resonance, ...)
- 585 • Environment (temperature, pressure, ...)
- 586 • Others (evaluation of data, publication, magic numbers, solvation-effect, ...)

587 The most important returned data will be mass spectra (which can also be visualized in a browser).  
588 Published papers related to the species asked for as well as possible evaluation programs [149] and  
589 their output will be made available. Larger files will be available by a download link found in the  
590 XSAMS data file (see par. 3.1.1). Since 1986 a group in Innsbruck [150,151] has been producing mass  
591 spectra of clusters via different approaches. These results are planned to be made available in this  
592 database.

### 593 3. Current Status of VAMDC e-Infrastructure

#### 594 3.1. Overview of the VAMDC e-Infrastructure Components

595 The e-infrastructure currently connects, in an interoperable way, 38 heterogeneous databases with  
596 atomic and molecular data. By providing data producers and compilers with a large dissemination  
597 platform for their work, VAMDC successfully removes the bottleneck between data producers and  
598 the wide community of atomic and molecular data users. The “V” of VAMDC stands for “virtual”  
599 in the sense that the e-infrastructure itself does not contain the data: it is a wrapper that exposes the  
600 heterogeneous databases in a unified way. The wrapping software, called the node-software [152],  
601 integrates a stand-alone database into a VAMDC federated database to become a data-node. Each  
602 data-node accepts queries submitted in a standard grammar (see Section 3.1.1) and provides output in  
603 a standard format. Each data-node is entered into the VAMDC registry (see Section 3.1.2) that enables  
604 a standardised application programming interface (API) to discover the available resources.

#### 605 3.1.1. Data Nodes, Query Language and Data Formats

606 A data-node is a database, either pre-existing or created for the purpose of VAMDC, wrapped in  
607 the node-software that implements the web-service<sup>43</sup> protocol VAMDC-TAP, which is derived from  
608 the International Virtual Observatory Alliance (IVOA)<sup>44</sup> Table Access Protocol (TAP).<sup>45</sup>

609 All VAMDC-TAP services support a common data model, query language and output format.  
610 The data model, expressed in the VAMDC Dictionary, represents the data both in a tree structure and

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<sup>43</sup> In this context, a *web service* is a data source on the WWW designed for access by application software. C.f. a *web page* designed to be interpreted by a human intellect.

<sup>44</sup> <http://ivoa.net/>

<sup>45</sup> <http://www.ivoa.net/documents/TAP/20190927/> TAP enables an application to query a remote database.

611 as a standardised set of virtual tables. The query language VAMDC SQL Subset 2 (VSS2)<sup>46</sup> operates on  
612 these virtual tables. The common output format is the XML Schema for Atoms, Molecules and Solids  
613 (XSAMS)<sup>47</sup> [153] that uses the tree-structured form of the data model. All VAMDC-TAP services  
614 allow XSAMS output while the nodes may optionally support other formats. XSAMS is highly flexible  
615 and expressive, but other formats may be preferred for compactness.

616 Libraries in Python of the node software are provided by the VAMDC consortium. The node  
617 owner configures these libraries for the database of choice by adding small translation-functions from  
618 VSS2 to SQL operating on the actual database, and from the query results to XSAMS or other formats.  
619 Additional information and examples of best practices were described by Regandell et al. [152].

### 620 3.1.2. Registry

621 The VAMDC metadata registry<sup>48</sup> lists the details of the VAMDC data-nodes. Applications use the  
622 registry to decide which databases should be queried and to locate the services for those databases  
623 on the internet. The VAMDC registry is based on the work of Astrogrid, which was the UK's Virtual  
624 Observatory development project from 2001 to 2010 [154]. They developed a registry whose interface  
625 is based on the then-current IVOA standard. To simplify the access to this registry, the VAMDC  
626 consortium provides Java and Python libraries that are used by the VAMDC portal, among other  
627 applications.

### 628 3.1.3. The Portal

629 The VAMDC portal<sup>49</sup> [155] relies on the infrastructure elements previously described in this  
630 section to provide seamless access to the inter-connected VAMDC databases. Through this unique  
631 interface a user can query any database member of the VAMDC infrastructure and can retrieve data in  
632 the common shared file format VAMDC-XSAMS (see Section 3.1.1). The page displaying the resulting  
633 data recalls the exact query processed by the infrastructure to produce the data (for example, see  
634 Fig. 1).

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46 <http://vamdc.eu/documents/standards/queryLanguage/vss2.html>

47 <https://standards.vamdc.eu/#data-access-protocol-query-language-and-dictionaries>

48 <http://registry.vamdc.eu/registry-12.07/main/index.jsp>

49 [https://portal.vamdc.eu/vamdc\\_portal/home.seam](https://portal.vamdc.eu/vamdc_portal/home.seam)

The screenshot shows the VAMDC portal interface. At the top is the VAMDC consortium logo. Below it is a navigation bar with links: Home, VAMDC databases, Guided query, Advanced query, Saved queries, Disclaimer, Citation policy, Privacy policy, Info, Tools, Login, Register. The main content area is divided into several sections:

- Query Execution:** A status bar shows 'Done' with a yellow progress bar. Below are buttons for 'Modify query', 'Stop waiting', and 'Save query'.
- Comments:** An empty text area for user comments.
- Your request:** A text box containing the SQL query: `select * where ((InchiKey = 'UGFAIRIUMAVXCW-UHFFFAOYSA-N'))`.
- Results by node:** A table with the following columns: Name, View data, Response, Last database update, Download, Species, States, Processes, Radiative, Collisions, Non Radiative.
 

Name	View data	Response	Last database update	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
SpEctroScopy of Atoms and Molecules	-- Choose display --	OK	11/04/2019 00:00	XSAMS file	1	1459	2000	2000	0	0
Water internet Accessible Distributed Information System	-- Choose display --	OK	05/11/2015 19:00	XSAMS file	1	320	1000	1000	0	0
UMIST Database for Astrochemistry	-- Choose display --	OK	Not available	XSAMS file	223	0	408	0	408	0

**Figure 1.** Example of the displayed results by the VAMDC portal after performing a given query. The processed query is highlighted in the *Your Request* box

635 The portal embeds processors to convert data from the XSAMS format into several formats  
 636 (chosen by user) and has several graphical tools to visualise the extracted data. Moreover, the portal  
 637 implements the IVOA-SAMP protocol [156] created to connect scientific tools when working with  
 638 multiple data types. VAMDC data can be directly piped from the portal into any tool implementing  
 639 the SAMP protocol, e.g. TOPCAT<sup>50</sup>.

### 640 3.2. Services Built over Existing VAMDC Infrastructure since 2016

#### 641 3.2.1. The Species Database

642 To overcome the problem of species identification, the VAMDC consortium created in 2016 a  
 643 centralised chemical-species repository called the species database. Updated daily by automated  
 644 collation of data from the VAMDC data-nodes, it contains the list of all the species in each VAMDC  
 645 database. Every species is identified uniquely by an InChIKey [157], a hash code generated from an  
 646 InChI description<sup>51</sup>. In the species database each InChIKey is associated with the different ways of  
 647 identifying a species; e.g. their chemical names, formula, stoichiometric formula and CAS number. By  
 648 adding a REST API and a web graphical interface to this species database<sup>52</sup>, we provide a versatile  
 649 tool to explore the species content of the atomic and molecular VAMDC connected databases. Using  
 650 this REST API<sup>53</sup> of the species database, the VAMDC portal provides both an autocomplete suggestion  
 651 for species names and identifiers and a feature to discover the isotopologues of a species. Thus, it is  
 652 possible to specify, very precisely, which species is the most relevant to a user's search.

<sup>50</sup> <http://www.star.bris.ac.uk/~mbt/topcat/>

<sup>51</sup> <https://iupac.org/who-we-are/divisions/division-details/inchi/>, <https://iupac.org/who-we-are/divisions/division-details/inchi/>

<sup>52</sup> <https://species.vamdc.eu>

<sup>53</sup> A RESTful API is an interface between a web-based client and a server that exploits [representational state transfer \(REST\)](#) constraints.

### 653 3.2.2. The Query Store

654 By using the VAMDC facilities, scientists can easily discover the atomic and molecular resources  
655 and access their data in a unique and practical way. However, as VAMDC has been adopted by a larger  
656 range of communities it has revealed a new set of challenging issues linked with citation and data  
657 reuse:

- 658 • The VAMDC infrastructure data are dynamic. A database displayed through the VAMDC  
659 infrastructure may evolve over time: the most recent and precise version of given data may  
660 replace old ones. We therefore needed mechanisms to allow the citation of dynamic data.
- 661 • The data set provided by the VAMDC infrastructure always contains the references of the papers  
662 used for compiling the data sets. However, the citation process may become cumbersome when  
663 the extracted data sets come from many sources.

664 VAMDC is addressing these issues at the data-community level and in 2014 VAMDC joined  
665 the Research Data Alliance. The RDA, through its [Data Citation Working Group](#) and [RDA/WDS  
666 Scholarly Link Exchange](#) (Scholix) Working Group, has defined new citation models in the digital era.  
667 We succeeded in implementing the RDA recommendations to provide the VAMDC users with a Query  
668 Store [158], a tool to facilitate citation of the data extracted from VAMDC for scientific reproducibility  
669 and for giving due credits to data producers. Through the Query Store:

- 670 • each query served by the infrastructure is identified by a persistently unique resolvable identifier;
- 671 • the query-produced data may be assigned a DOI<sup>54</sup>;
- 672 • data become directly citable by their DOI.

673 When registering a DOI, the authors of the papers used for compiling the data appear in the "references"  
674 part of the DOI-metadata schema. The data-set sources become the references of the DOI. The  
675 authors/papers referenced in the VAMDC extracted data set will automatically get credit when the  
676 data set is cited (using the DOI) into a paper.

677 Table 2 lists the VAMDC databases currently integrated with the Query Store service, whose  
678 queries may be discovered by accessing the URL<sup>55</sup>; this service is the most complete collection of  
679 VAMDC queries that may be cited as example of the queries performed through the infrastructure.

**Table 2.** List of databases connected with the Query Store service. The databases marked with a star (\*) are currently being connected to the Query Store and the test phase is in progress.

VALD	Topbase	Tipbase
SHeCaSDa	MeCaSDa	GeCaSDa
TFMeCaSDa	RuCaSDa	TFSiCaSDa*
UHeCaSDa*	ECaSDa*	Stark-B
CDMS	JPL	BeamDB
Mold	SeSAM	Basecol*

### 680 3.3. Pending Technical Issues

681 In addition to all of the advancements of the individual databases and VAMDC as a whole, there  
682 are still technical issues that need to be addressed in the future.

#### 683 3.3.1. Treatment of Big Data

684 The growth in large data sets, which is common to all areas of science, is also true in A&M  
685 physics. VAMDC uses a tightly defined and rigorous data structure that is also, as a result, relatively

<sup>54</sup> DOI: [Digital Object Identifier](#), a formal name for a document or data-set in a standard format intelligible by software.

<sup>55</sup> <https://cite.vamdc.eu>

686 verbose. This means that the data returned by queries to some databases such as VALD and KIDA  
687 are already limited by the software so as not to cause problems. Moreover, if many current VAMDC  
688 molecular spectroscopic databases contain data with a relatively limited amount of spectral lines for  
689 each molecule (HITRAN, JPL, CDMS, . . .), some others (MeCaSDa, . . .) contain extensive calculated  
690 line lists, and in this case, their number for a given species can be very large (several millions of spectral  
691 lines at least) and could increase even more with subsequent updates. At present there is a limit within  
692 the VAMDC data retrieval volume. Queries producing large data extracts time out or are truncated by  
693 the data-nodes to avoid timeouts. This prevents downloads of line lists over a wide spectral range or  
694 for many molecules at once. The actual limits vary from node to node according to the computing  
695 resources invested and the details of the database.

696 For example, when asked for all data connected with lines between 150 nm and 800 nm, seven  
697 nodes produced a complete result, three produced a truncated result, two failed and one timed out;  
698 the others quickly reported that they had no relevant data. The largest response was for 67 million  
699 lines in 218MB of XSAMS, and this is close to the practical limit of the system. For this data-set, three  
700 of the recommended displays and format-converters were able eventually to process the data, one  
701 failed and one produced no results within 10 minutes.

702 This is a problem for applications in atmospheric planetary physics and exoplanet studies. A  
703 solution currently under investigation is the possibility of asynchronous queries that run slowly in the  
704 background and leave their results cached and accessible by an ephemeral URL.

705 There are also whole databases that are currently really too big to be usefully probed via the  
706 VAMDC portal. A particular area that produces very large data sets is the provision of molecular line  
707 lists for studies of hot atmospheres. The ExoMol [126,127], TheoReTS [159] and the NASA Ames group  
708 (e.g. [160]) all employ theoretical methods to compute very extensive lists of molecular transitions  
709 particularly for high-temperature applications in astrophysics. Many of these line lists are huge;  
710 for example, the ExoMol line list CH<sub>3</sub>Cl contains 166 billion transitions for each of the two main  
711 isotopologues [161]. Even at room temperature, complete line lists for relatively heavy long-lived  
712 greenhouse molecules with low-frequency vibrations like CF<sub>4</sub> [162] or NF<sub>3</sub> [163] require billions of  
713 transitions to converge opacity calculations over infrared wavelengths. Data sets of this size are  
714 completely outside the current capabilities of the VAMDC project.

715 Some work has been performed on data compacting, in particular using the so-called super-lines  
716 approach [164,165]. Another method of big-data compression is to use “effective” lines as implemented  
717 in a recent addition of methane [89] to the HITEMP database [86]. Use of these protocols can lead to a  
718 very significant reduction in the size of the effective line list, but these compressed lists still contain  
719 many millions of lines making it difficult for the current VAMDC infrastructure to process or download  
720 the full line list even after it is compacted. We note that the ExoMol line lists have recently been used to  
721 generate a set of temperature and pressure dependent opacities [37] creating the so-called ExoMolOP  
722 database. These opacity functions provide a much more compact representation of the molecular  
723 data, and an implementation of the ExoMolOP database within VAMDC is currently being explored.  
724 A similar direction is currently being followed for the TheoReTS information system<sup>56</sup> containing a  
725 theoretical and experimental atlas of methane absorption/emission cross sections [166] up to 1000 K.

### 726 3.3.2. Selection and Comparison of Atomic States

727 It is a long-standing goal of VAMDC to be able to combine data from different databases that  
728 relate to a given state or energy level of an atom or molecule. This allows comparison of measurements  
729 or theoretical values from different sources, and also permits a fuller set of data to be built up: e.g.  
730 energies for radiative transitions from one database combined with broadening values from another.  
731 This comparison needs a common labelling-scheme for states and energy levels.

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<sup>56</sup> <http://theorets.univ-reims.fr>, <http://theorets.tsu.ru>

732 This common labelling is already achieved for simple molecules in the “case by case” formalism  
733 of XSAMS. The tool SPECTCOL [109,110], which takes spectral data from CDMS and collisional  
734 excitation rates from BASECOL, exploits this. The labelling of states simplifies the current, theoretical  
735 understanding of the molecules sufficiently for the software to suggest states that *might* be treated as  
736 equivalent: i.e. it performs a “fuzzy” match from which an expert user can pick states to treat as true  
737 matches.

738 It is currently much harder to combine data on atomic states and levels. This part of the  
739 XSAMS data-model allows greater precision and flexibility in the description of a level at the cost of  
740 easy matching between databases. We hope to retain the current accuracy of the data model while  
741 augmenting it with extra notations that are less precise but more consistent between databases. Thus  
742 we may recover the ability to make “fuzzy” matches between databases. The restricted notations  
743 introduced by the PyValem software-package<sup>57</sup> may be relevant here.

744 We emphasize that we are not seeking *exact and complete*, quantum-mechanical descriptions of  
745 all states. We understand that such a description may not be possible with the current, theoretical  
746 models of atoms, which are themselves approximate and incomplete (except for the simplest atoms).  
747 Furthermore, state descriptions precise to the limits of current theory may not be unique e.g. due to  
748 underlying assumptions about coupling and state mixing. Thus, the VAMDC consortium is exploring  
749 hierarchical structures for describing atomic terms and electronic configurations. At the highest,  
750 most-precise level, these would describe the atoms to the full extent allowed by current theory. At the  
751 lower, more-approximate levels, they would allow automatic matching of data that probably describe  
752 the same states, leaving final interpretation to expert users. As a bonus, we hope to make it possible to  
753 select from the databases just the data relating to particular atomic levels and states.

### 754 3.3.3. Update of Node-Software

755 The common Python software on which most data-nodes are built relies on a small suite of  
756 third-party libraries. We wish to keep this infrastructure baseline constant as long as possible to  
757 enhance stability and reduce maintenance for the node operators. However, it is now necessary to  
758 upgrade to newer versions of the libraries. Notably, Django<sup>58</sup> v2, which is no longer supported, must  
759 be replaced with v3. This may force some changes in the customisation of each node since Django  
760 upgrades are rarely compatible in all APIs.

761 Provided that old and new versions of the node-software support the same version of VAMDC  
762 standards, we do not require all the data-nodes to be upgraded at the same time.

## 763 4. Applications and User Case Studies

764 Any database lives from the use of its data, the more the better. Many applications need concerted  
765 access to different databases, just what is provided through VAMDC. Here, we present a few of these  
766 applications that demonstrate the use and benefit of VAMDC.

### 767 4.1. CASSIS Software

768 CASSIS<sup>59</sup> (Centre d’Analyse Scientifique de Spectres Instrumentaux et Synthétiques) is a  
769 standalone software written in Java, freely delivered to the community for help in visualising, analysing  
770 and modelling observations from ground or space-based observatories. It has been developed at IRAP  
771 since 2005 and is part of the OVGSO data centre that aims at promoting VO technology. It displays  
772 any spectra (ASCII, FITS or GILDAS/CLASS format or the result from a query to any SSAP<sup>60</sup> VO or

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57 <https://github.com/xnx/pyvalem>

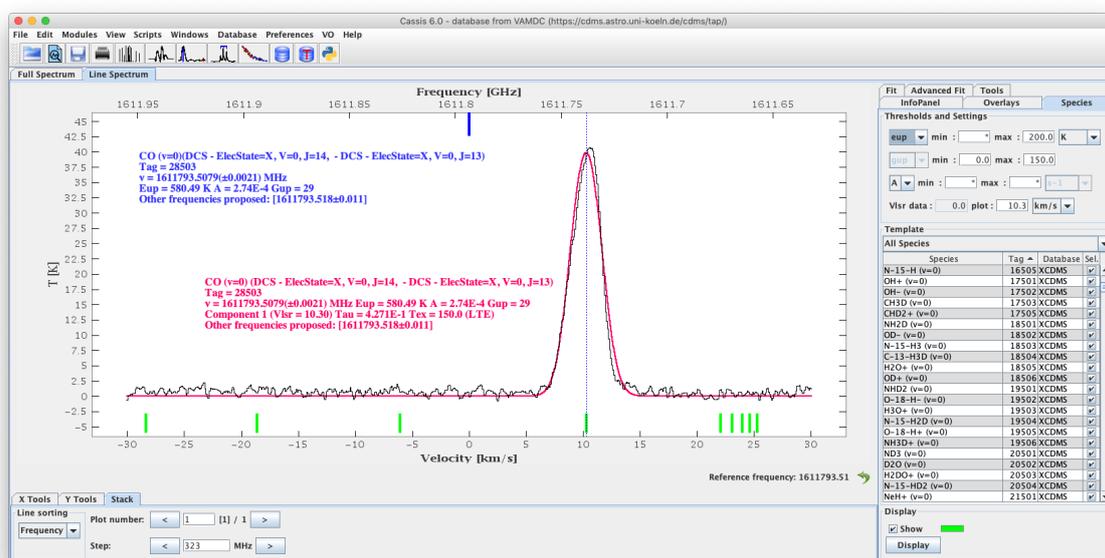
58 <https://www.djangoproject.com/>

59 <http://cassis.irap.omp.eu>

60 <http://www.ivoa.net/documents/SSA/20120210/>

773 EPN-TAP[167] VO service from IVOA registries) and identifies atomic and molecular species through  
 774 its link to databases such as JPL [15] and CDMS [74] via a SQLite database. Species identification may  
 775 also proceed via a direct access to VAMDC for any available spectroscopic database using TAP (the  
 776 Table Access Protocol), which is based on the IVOA format.

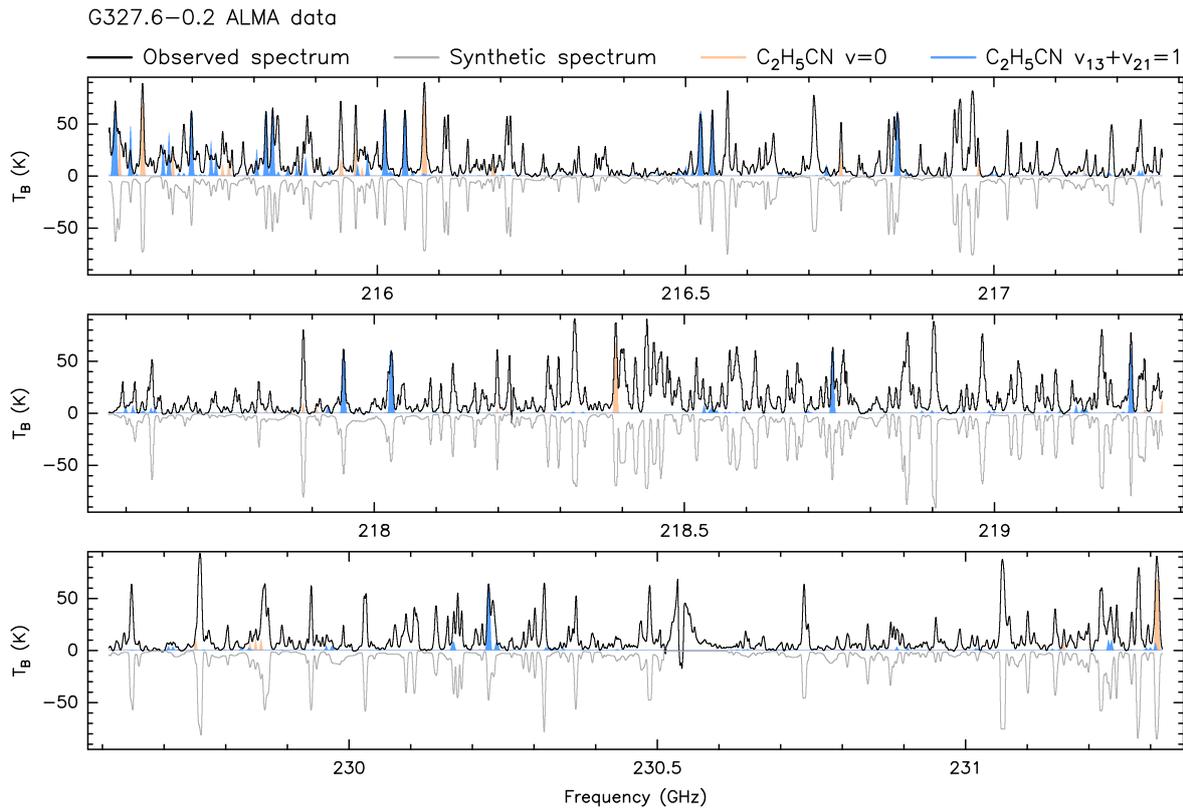
777 Modelling is performed in Kelvin units, and a conversion tool for Jansky units is available. LTE  
 778 (Local Thermodynamic Equilibrium) and non-LTE modelling tools are provided. CASSIS gives  $\sim 80$   
 779 collision files constructed from the LAMDA [168] and BASECOL [29,30] databases, as well as from local  
 780 files, such that their quantum numbers, Einstein coefficients, upper energy levels and rest frequencies  
 781 match the request made within CASSIS. Indeed, some molecular species appear both in JPL and CDMS  
 782 with sometimes different spectroscopic parameters, hindering the request for the modelling of line  
 783 profiles. In the near future CASSIS will use the SPECTCOL tool [109,110], developed by the VAMDC  
 784 consortium, to associate spectroscopic data provided by spectroscopic databases with collisional data  
 785 provided by collisional databases to obtain the most up-to-date rate coefficients. Analysis modules for  
 786 line and baseline fitting, resampling, rotational diagram analysis and  $\chi^2$  minimisation with Jython<sup>61</sup>  
 787 scripts are available to find best-fit model parameters such as column density,  $T_k$  (or  $T_{ex}$ ),  $n(\text{H}_2)$  or  
 788 source size.



**Figure 2.** Example of a request made within CASSIS for an observed transition of CO (black) using the CDMS node of VAMDC for the line identification and LTE modelling (red) (see text). The right side of the figure shows the species available in the database and the possible thresholds on the Einstein coefficients and upper energy levels. The  $V_{LSR}$  is also given for the shift applied to the databases' frequencies, and the green bars below the spectrum correspond to the possible transitions within the frequency range.

789 Fig. 2 shows an example of an observed spectrum (in black) of a CO transition compared with  
 790 LTE modelling (red) of the CO transition using the CDMS node in VAMDC. The vertical blue bar  
 791 corresponds to the requested CO transition unshifted for the  $V_{LSR}$  (velocity in the standard of rest).  
 792 The vertical green bars correspond to the transitions that appear in VAMDC with the thresholds on  
 793 the upper energy levels and Einstein coefficients, and shift in  $V_{LSR}$  (right side of the Figure). The  
 794 spectroscopic parameters are listed in blue for the observations and in red for the model with the

<sup>61</sup> <https://www.jython.org>



**Figure 3.** Spectra towards the high-mass star-forming region G327.3-0.6, with the intensity in brightness temperature unit ( $T_B$ ) observed with the Atacama Large Millimeter/submillimeter Array (ALMA). The myCLASSfit function was used to model the observational data shown in black. Synthetic spectrum including all identified molecular species are shown in grey, and has the intensity multiplied by a factor  $-1$ . This study aimed at finding and quantifying ethylcyanide ( $C_2H_5CN$ ) in these dense spectra. The contribution from  $C_2H_5CN$   $v=0$  and  $C_2H_5CN$   $v_{13} + v_{21} = 1$  transitions are highlighted in orange and blue, respectively (Reproduced from [169], Copyright Elsevier (2020)).

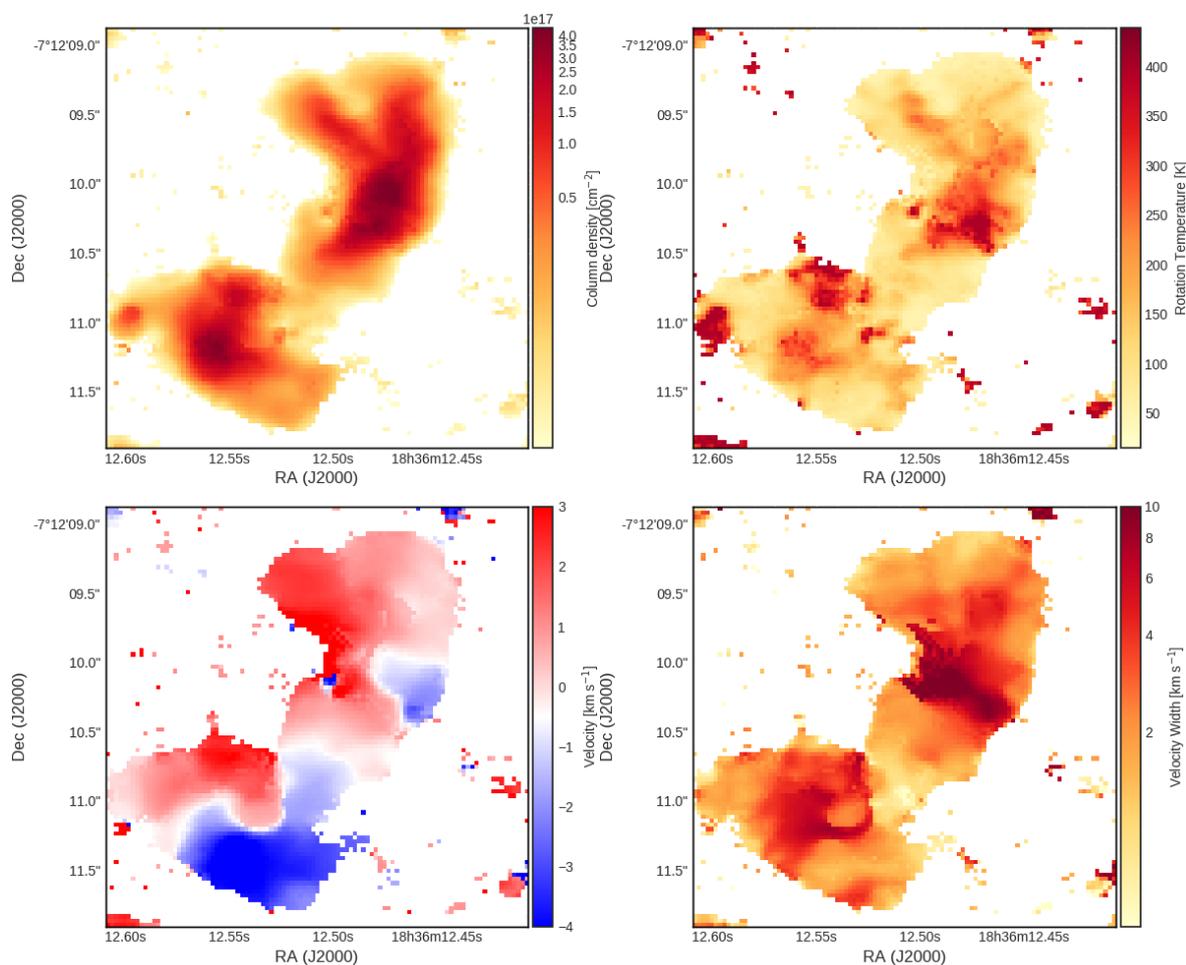
795 resulting opacity and excitation temperature values. When VAMDC proposes different frequencies for  
 796 a given transition (derived, predicted, experimental values) that may even originate from the same  
 797 database, CASSIS selects the frequency with the minimum uncertainty.

#### 798 4.2. XCLASS - eXtended CASA Line Analysis Software Suite

799 XCLASS<sup>62</sup> [170] is a full message passing interface (MPI) parallelised toolbox for the Common  
 800 Astronomy Software Applications package (CASA), aimed at fitting spectral line data from  
 801 astronomical sources observed both with interferometers or single dish telescopes. XCLASS models a  
 802 synthetic spectrum that is automatically compared to the data with the aim of providing a measurement  
 803 of physical quantities, such as the temperature, molecular abundance and velocity. Molecular  
 804 data required by XCLASS are taken from an embedded SQLite3 database containing entries from  
 805 CDMS [74] and JPL [15] that is populated and updated via the Python library VAMDCLIB, which queries  
 806 the data directly from the VAMDC nodes. XCLASS offers the possibility of describing molecules  
 807 and radio recombination lines (RRLs) in LTE and non-LTE conditions using the RADEX<sup>63</sup> formalism.  
 808 Hereby, local overlap of lines can be taken into account as well. Furthermore, non-Gaussian line

<sup>62</sup> <https://xclass.astro.uni-koeln.de/>

<sup>63</sup> <https://personal.sron.nl/~vdtak/radex/index.shtml>



**Figure 4.** Example of parameter maps created by the myXCLASSMapFit function using nine transitions of CH<sub>3</sub>OCHO simultaneously, taken from an ALMA data set of the core of G24.78 [172].

809 profiles such as Lorentzian, Voigt (including pressure broadening for RRLs) and Horn can be used.  
 810 Different continuum contributions like dust, free-free and synchrotron emissions can also be modelled.  
 811 Finally, complex source structures can be described by using sub-beam descriptions and component  
 812 stacking. The toolbox contains an interface for the model optimiser package MAGIX (Modelling and  
 813 Analysis Generic Interface for eXternal numerical codes) [171], which helps to find the best description  
 814 of the data using a certain model; i.e. finding the parameter set that most closely reproduces the data.  
 815 XCLASS can also automatically identify the molecules producing a given spectrum.

816 In XCLASS, the myXCLASSFit function can be used to fit multiple spectra, i.e. to fit multiple  
 817 frequency ranges simultaneously in multiple files (see Fig. 3). The function returns the optimised  
 818 model parameters and the corresponding modelled spectra.

819 In addition, the XCLASS interface contains the myXCLASSMapFit function that fits one or more  
 820 complete (FITS) data cubes. For this the myXCLASSMapFit function reads in the data cube(s), extracts  
 821 the spectra for each pixel and fits each spectrum separately. At the end of the whole fitting procedure,  
 822 the myXCLASSMapFit function creates FITS images for each free parameter of the best fit, where each  
 823 pixel corresponds to the value of the optimised parameter taken from the best fit for that pixel (see  
 824 Fig. 4). Some applications of this include temperature maps, as well as first and second moment maps,  
 825 which are based on the simultaneous fitting of many lines and are fairly robust against line confusion  
 826 and blending of single lines—this can be a severe issue in many ALMA data sets with line-rich sources.  
 827 The new CubeFit function is an extension to the myXCLASSMapFit function, and can be used to  
 828 describe data cubes by physical models.

### 829 4.3. Use of Stark-B Data

830 From an analysis of applications of Stark broadening parameters [173], calculated with a  
831 semi-classical perturbation method [68], it was shown that the main users of Stark-B data are  
832 astronomers, who use them for investigation of A and B type stars, white dwarfs and hot stars  
833 in late evolution stages, as for example PG1159 type stars<sup>64</sup> [174]. The data most often used for this  
834 purpose primarily concern He I and Si II. Additional usage of these data is for plasma modelling in  
835 physics and technology, primarily for laser produced plasma with some emphasis on Stark broadening  
836 parameters of Zn I. An analysis of the citations to the Stark-B database shows that its data are also  
837 used for different analyses of regularities and systematic trends, as a source of a large number of  
838 homogeneous data obtained in the same way [175]. The Stark-B database is often cited in studies of  
839 spectral lines within laboratory plasma.

### 840 4.4. Examples of Concrete User Issues

841 Through the federation of resources and the adoption of common standards, the key features of  
842 the VAMDC e-infrastructure are its ability to query all resources with the same type of queries and to  
843 retrieve data identified with the same metadata. Theoretically this is a very big step towards speeding  
844 the retrieval of data in a safe and secure way. As an example, through VAMDC it is impossible to  
845 make a mistake when querying a given atomic species with its given ionisation stage: all databases  
846 will return data concerning that specific query. On the other hand, it is easy to query the wrong  
847 ionisation stage by going directly to the different databases. For example, a question from a user was:  
848 "I searched  $\text{Ca}^+$  in the wavelength range from 4800 Å to 4950 Å directly from NIST, from VALD, and  
849 from VAMDC/NIST and VAMDC/VALD. None of the transition wavelengths seem to be identical,  
850 what shall I take?" It turned out that the user had in fact queried  $\text{Ca}^+$  in NIST and Ca in VALD. The  
851 VAMDC query was obviously the same both for VAMDC/NIST and VAMDC/VALD, but the values  
852 seemed to differ between NIST and VAMDC/NIST. It turned out that VAMDC transfers by default  
853 wavelengths in vacuum while a direct request to NIST provides wavelengths in air and direct request  
854 to VALD provides wavelengths in vacuum. This simple example shows the difficulty that users might  
855 encounter.

856 In spite of major advances developed by the VAMDC federation, we have identified several  
857 user issues of such an e-infrastructure, which in turn might prevent its wider adoption by several  
858 communities. Users have their habits with queries and output formats; to a lesser extent, they question  
859 the data directly obtained from the long-established databases. Databases sometimes offer science  
860 services that facilitate the users' work; for example, helping the user to choose the right set of the  
861 database's data for their application. Other databases may include recommendations of their own data  
862 whenever, for identical processes, the database contains different values. For example, the BASECOL  
863 database keeps historical collisional sets even when new data sets are included for the same process,  
864 and data sets are labelled as recommended or not. This local feature is not currently transferred  
865 through VAMDC.

866 Some knowledgeable users would like that the VAMDC portal provide the functionality to choose  
867 the databases prior to specific queries on species and processes, thus avoiding unnecessary waiting  
868 time. Users deploying applications such as CASSIS (Section 4.1) would appreciate the option to make  
869 total or partial copies of the databases locally in order to speed up their application. Such copies would  
870 be coupled to a rapid search for the availability of updates. Some users would appreciate a lighter  
871 format than the XSAMS format.

872 We can therefore identify the following non-exhaustive and general issues to address in the future:  
873 (i) trust in a new numerical environment; (ii) the ability to quickly understand and compare data;

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<sup>64</sup> It is the prototype of stars with a hydrogen-deficient atmosphere that is in transition between being the central star of a planetary nebula and a hot white dwarf, named after their prototype, PG1159-035.

874 (iii) the ability to choose the right data for its own usage and improvement/development of tools.  
875 Some of the future lines of work are outlined in Section 6. Closer collaborations between the VAMDC  
876 community and different user communities will be addressed through a VAMDC users committee  
877 whose representative will be part of our boards.

## 878 5. Current Impact of VAMDC on the Community

### 879 5.1. Node Data Standardisation and Quality Control

880 An interesting impact that VAMDC has on participating databases is the pressure to introduce  
881 accurate and complete descriptions of data elements stored on individual nodes. Such descriptions  
882 are necessary for uniform representation of A&M data in XSAMS. In practice the construction of the  
883 translation dictionary between the local node and XSAMS requires unambiguous interpretation of  
884 data elements. While this sounds trivial for physical parameters like energy and frequency, the task  
885 becomes increasingly more difficult when dealing with energy level classification, quantum numbers,  
886 mixed states, etc. For the nodes that store data compilations from different sources and authors (e.g.  
887 VALD) the connection to VAMDC provides a good motivation for setting internal standards. Without it,  
888 researchers maintaining the local node would be much less interested in spending time, for example, on  
889 converting or creating atomic energy level descriptions in the appropriate coupling scheme following  
890 the format that is unique and can be automatically analysed to get the main quantum numbers. Once  
891 this work is done, the XSAMS description of energy levels becomes straightforward. Standardisation  
892 also opens opportunities for verification of the basic QM selection rules, cross-comparison between  
893 data from different authors or/and data between nodes as well as trust assessment of expert data [176].  
894 Mistakes, typos and misinterpretations discovered in this process significantly improve the quality  
895 of the data products and reduce the amounts of errors introduced between data production and its  
896 extraction through the VAMDC portal. Standards introduced by VAMDC play a decisive role in this  
897 improvement, while the practical work of course falls on the shoulders of people maintaining local  
898 nodes.

### 899 5.2. VAMDC and the FAIR Principles

900 VAMDC experts have been involved for several years in international data-sharing organisations  
901 (see Section 5.5) and have anchored *ante-litteram*<sup>65</sup> the FAIR Principles [177] into the design of the  
902 VAMDC infrastructure. The FAIR principles are implemented with a fine-grained granularity:

- 903 • Findable: data coming from the infrastructure are assigned persistently unique identifiers  
904 (Section 3.2.2), are described by rich metadata schemes and are indexed into public registries  
905 (Section 3.1.2).
- 906 • Accessible: the extraction query relies on open, documented standards (Section 3.1.1).
- 907 • Interoperable: the data extracted from VAMDC are formatted using the XSAMS standard  
908 (Section 3.1.1). Moreover VAMDC implements widely adopted international data-interoperability  
909 standards (Sections 3.1.3 and 3.2.2).
- 910 • Re-usable: the provenance and sources of all the data are documented in each data set extracted  
911 from VAMDC. Data tools are provided to convert VAMDC data into widely adopted community  
912 data formats (Section 3.1.3).

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<sup>65</sup> An early definition of the Findable, Accessible, Interoperable and Reusable (FAIR) principles was given by Larry Lannon from CNRI in 2012 when he introduced the DAIR principles: the D standing for Discoverable will be replaced by the F for Findable.

### 913 5.3. Development of New Software, Databases and Portal

#### 914 5.3.1. GrafOnto Collection of Scientific Plots

915 The construction of databases, extracted from tabular resources in spectroscopy, required VAMDC  
916 to pay attention to the spectral functions presented in the form of plots and figures. The basis for  
917 creating a database of spectral functions was a digital library of more than a thousand articles with  
918 plots and figures, containing spectral functions for the problem of continuum absorption [178], the  
919 properties of weakly bounded complexes, including atmospheric molecules [179] and the absorption  
920 cross sections in the near and far ultraviolet ranges. In these subject domains the amount of graphical  
921 information is much larger than the amount of tabular information. We identified typical examples of  
922 plots and figures under study and created ontologies [105] of graphical resources, tools for integrating  
923 plots and means for citation quality assessment [107].

924 At present the collection contains about 3500 original and 1055 cited primitive plots combined  
925 into 980 composite plots and 166 composite figures. The uploaded plots describe the properties of 19  
926 molecules, 44 complexes and 66 mixtures. 2338 primitive plots characterise the properties of a water  
927 molecule and water dimer. The GrafOnto graphics system is available at its URL<sup>66</sup>.

#### 928 5.3.2. New On-Line Databases and Community Portal

929 The VAMDC project has directly stimulated the creation of new online databases such as  
930 TFSiCaSDa and UHeCaSDa [19], and the deployment of the theoretical PAH database within VAMDC  
931 [3,36] while motivating the development of an experimental databases for PAHs. The VAMDC  
932 infrastructure deployment also encouraged a similar strategy for experimental databases for solid-state  
933 data in SSHADE (Section 2.3.2). Collaborations with VAMDC directly led to a renewed effort to compile  
934 local data in India (see Section 2.3.5). The RADAM collaboration adopted the VAMDC standards and  
935 designed a RADAM portal<sup>67</sup> that offers access to the VAMDC connected databases in addition to some  
936 other databases to their community.

937 The Belgian repository of fundamental atomic data and stellar spectra (BRASS) [180]—which  
938 aims to provide the largest systematic and homogeneous quality assessment of atomic data to date  
939 in terms of wavelength, atomic and stellar parameter coverage—retrieved atomic data from various  
940 repositories and cross-matched these data. The majority of repositories were queried using the VAMDC  
941 e-infrastructure and the BRASS consortium thus acknowledged the efforts of the VAMDC team in  
942 homogenising the repositories as this has helped to expedite their comparisons and cross-match work.

### 943 5.4. Sustainability Issues

944 Today's science often seeks to treat complex applications such as the modelling of planetary  
945 atmospheres. The large amount of data needed to make realistic simulations is in sharp contrast to  
946 what a single researcher or institution is able to collect. Therefore, there is a common need and interest  
947 for large repositories of data and their accessibility by the community. Thus the need of sustainability  
948 of scientific data has been understood also by funding agencies and, on a larger scale, by science  
949 policy makers. All national and international calls for scientific projects now routinely demand that  
950 applicants provide a sustainable way to make validated scientific data from the project available to the  
951 general community for the long term, often specifying open access.

952 The sustainability issue occurs on different levels. At the lowest level, original data from laboratory  
953 measurements, computations or field measurements, e.g. astronomical observation data, are stored in  
954 a repository such that at least their validity can be checked after many years. The next level concerns

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<sup>66</sup> <http://wadis.saga.iao.ru/rdf/plot/plot.rdf/>

<sup>67</sup> <http://radamdb.mbnresearch.com/#>

955 processed data being kept in a certain format to become available for later analysis to avoid unnecessary  
956 repetitions of work. All this requires a minimum level of documentation in order to retrieve the data.  
957 In that respect, association of data with a DOI or other identifiers is currently being developed and  
958 becoming available on national and international levels, but it requires infrastructure and organisation  
959 down to the level of individual institutions. Common standards such as the DOI are important means  
960 to reach a reasonable level of documentation and accessibility.

961 Databases connected to VAMDC offer a reliable and established way of supplying even further  
962 processed data, and therefore, are one of the most advanced answers to the concern of sustainability.  
963 The VAMDC consortium has agreed common standards and descriptions, which serve as a one-shop  
964 place for a plethora of atomic and molecular data. By defining common schemes for the data stored in  
965 the various databases, VAMDC has reached an invaluable level of interoperability and, therefore, a  
966 unique level of sophistication. VAMDC is an open platform that welcomes databases from all over  
967 the world and, as such, provides a focal point of atomic and molecular data. As a result, VAMDC  
968 serves as a role model to structure research data on international, national and local levels. We can cite,  
969 for instance, the DAT@OSU portal that gathers metadata for all research databases in the Bourgogne  
970 Franche-Comté region in France [181].

971 Sustainability issues are also related to human training and capabilities. In that respect, VAMDC  
972 has trained engineers and post-docs who are still involved in the fields of software developments,  
973 database management, development of standards for the benefit of the public sector in the VAMDC  
974 collaboration and in other domains, as well as in the private sector.

#### 975 5.5. Impact on Open Science Initiatives and International Data Alliances

976 VAMDC delegates are active and have a high reputation in international data alliances, where  
977 they bring the VAMDC requirements and expertise about open-data sharing:

- 978 • VAMDC has been active in the [Research Data Alliance](#) since 2014 (Section 3.2.2), when  
979 VAMDC became an early pilot for the *data-citation recommendation*. Starting from 2016  
980 VAMDC took a leading role in the [RDA-Federated Identity management Interest Group](#): the  
981 RDA-recommendations produced by this interest Group [182] incorporate ideas and needs  
982 coming from the *Authentication, Authorisation and Accounting strategy* we developed for the  
983 VAMDC Consortium [183].
- 984 • Since 2016, we have worked with the [IVOA](#) on converging VAMDC and the IVOA atomic and  
985 molecular standards<sup>68</sup>.

986 The current *Executive Director* of the Consortium represents VAMDC in the [Group of European Data](#)  
987 [Experts](#) in RDA (GEDE-RDA), and is one of the two co-chairs of this group. The aim of GEDE-RDA  
988 is to promote, foster and drive the discussions and consensus forming on creating guidelines, core  
989 components and concrete data fabric configuration building based on a bottom-up process. To achieve  
990 these goals, GEDE-RDA is composed of a group of European data professionals appointed by invitation  
991 from various European Research Infrastructures and some specialists from the Research Data Alliance.  
992 The core group includes delegates from 47 European research infrastructures. The chairs from the  
993 European Strategy Forum on Research Infrastructures (ESFRI) and the e-Infrastructures Reflection  
994 Group (eIRG) agreed to take an observation role. Through our participation in GEDE-RDA, the  
995 VAMDC experience and vision directly contribute to the definition of international standards [184]  
996 and to the definition of the European Open Science agenda [185]. Since November 2019, the VAMDC  
997 Portal, the Species Database and the Query Store (see, respectively, Sections 3.1.3, 3.2.1 and 3.2.2) have  
998 been registered as parts of the European Open Science Cloud (EOSC) hub and VAMDC is a service  
999 provider for the [EOSC Market-Place](#).

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<sup>68</sup> <http://www.ivoa.net/documents/SLAP/>, <http://www.ivoa.net/documents/SLAP/>

1000 Our involvement in *Open Science* has been acknowledged at the French National level, where the  
1001 VAMDC executive director has been invited to join the [The Research Data College](#), which is responsible  
1002 for defining and implementing the French Open Science data agenda.

## 1003 6. Visions of the Future

1004  
1005 When the VAMDC project was first conceived the thinking was that if we could introduce a strict  
1006 and complete standard for describing atomic and molecular data, work out the transport protocol,  
1007 the (standard) interface to the individual nodes and the common user portal, it would solve most  
1008 of the problems limiting user access to the variety of data collections and data formats available on  
1009 the web. VAMDC has made enormous progress in establishing the XSAMS standard for describing  
1010 energy levels in atomic and molecular species, the node-software with its dictionaries for quick and  
1011 reliable interfacing to the individual nodes and the portal. VAMDC introduced a registry for the  
1012 regular indexing of node status and data content, publishing tools to encourage data providers to  
1013 publish new data in VAMDC, query storage and many other tools. Essentially all the initial goals  
1014 have been achieved and we have demonstrated all the functionality and reliability aspects of the new  
1015 infrastructure.

1016 Now, after several years of using and promoting VAMDC to other users, we see that our original  
1017 goals, while ambitious, were not sufficient to make VAMDC the ultimate source of A&M data. The list  
1018 of problems that an average VAMDC user is facing includes difficulties in automatically analysing  
1019 XSAMS files, restriction on their size, complications in cross-identification between XSAMS generated  
1020 by different nodes, and some missing functionality offered by the nodes through their native interfaces,  
1021 etc. Thus, the work on VAMDC is far from complete, but it has a strong foundation and an extensive  
1022 toolbox that can be built upon in the future.

1023 In order to enhance the usefulness of the VAMDC system in the delivery of A&M data to a wider  
1024 community of users, VAMDC needs a more "understanding" interface, much more flexible means  
1025 for extracted data manipulation and new complex data selection constraints, for example, based on  
1026 models of the environment. In the following sections we discuss our plans to develop VAMDC in the  
1027 future.

### 1028 6.1. User Interface

1029 Our attempts to be very precise in describing atomic and molecular configurations with XML  
1030 schema have had an unexpected adverse effect on the user interface implemented in the portal. At  
1031 first sight the portal seems to have an amazing flexibility: one can start from specific energy levels  
1032 or processes, but the flexibility is massively reduced by the rigidity of the XSAMS requirements  
1033 and "restrictables"<sup>69</sup> supported by each node. The only field that has some rudimentary attempt in  
1034 translating user input into alternative representations is the field "species" that allows auto-completion.  
1035 This is made possible through the species database described in Section 3.2.1. In the future VAMDC  
1036 will explore the possibility of creating/adopting an engine for interpretation of much more relaxed  
1037 formulations of the user's request, using iterations gradually narrowing the requested data set to the  
1038 user's needs. This more intuitive approach is complemented by the final query format available to the  
1039 user (e.g. through the Query Store described in Section 3.2.2) allowing for quick automation of the  
1040 process.

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<sup>69</sup> Restrictables refer to the data types for which selection criteria can be included in the VAMDC query, <https://standards.vamdc.eu/dictionary/restrictables.html>

## 1041 6.2. Complex Restrictions in VAMDC Request

1042 Allowing for fuzzy definitions in the user interface through the portal may (and will) require  
1043 additional levels of complexity in the request. For example, the interaction with the user may result in  
1044 more than one complementary requests to be previewed before making a final decision. This can be  
1045 further extended to the model-based selection, when constraints are set on properties sensitive to the  
1046 environment, for example, spectral line strengths in the Earth atmosphere or in a given experimental  
1047 or industrial setup. Estimating such derived properties requires additional information, such as the  
1048 equation of state and partition functions, which at the moment are not offered through the VAMDC  
1049 interface. Another example of such a complexity layer that could be useful is the ability to select  
1050 multiple processes such as Raman transitions. Some molecular databases contain Raman transitions  
1051 (e.g. MeCaSDa and SHeCaSDa).

## 1052 6.3. Large Data Sets

1053 As discussed above, the current VAMDC portal is not designed to easily handle databases with  
1054 many millions or even billions of transitions. At the smaller end of these, it is possible to include the  
1055 database but limit the amount of data that can be downloaded. At present really large databases are  
1056 simply excluded. A possible solution could be to allow asynchronous queries followed by an e-mail  
1057 sent to the user with a link to the result.

1058 More concise data sets may require sacrificing the completeness of XSAMS. Formats that represent  
1059 projections of XSAMS structure onto a single or multiple tables, independent tables such as FITS  
1060 are not able to carry complex inter-relations of the data model. Indeed, FITS is an open standard  
1061 mainly designed for image transport (as its name indicates). It may still be used in specific cases when  
1062 requested data can be arranged in a table, for example a line list with data for computing opacity  
1063 tables. In this case the FITS headers could provide the metadata explaining the meaning of numerical  
1064 elements. In more general cases the complexity of relations in atomic and molecular physics calls for  
1065 tree-based formats like XSAMS, that is a graph oriented data model.

1066 Relational sets of tables could be the right compromise. The most concise but generally useful  
1067 format may be an SQLite file containing the query results in the form of an independent, relational  
1068 database. Supplying extracted data as miniature databases also provides an easy way to query within  
1069 the data subset stored on the users' own computers. SQLite is a well-established tool with widespread  
1070 support in scientific computing. Ultimately, this approach allows a user to obtain a database that is a  
1071 cached copy of the data in a VAMDC node, and that can readily be refreshed from that node as data  
1072 are added or changed in the node. The VAMDC infrastructure will be developed to support these  
1073 cached copies and to embed them into applications, as has been demonstrated in the user case studies  
1074 discussed above in Section 4.

## 1075 6.4. XSAMS Manipulation

1076 We have previously considered creating a library for XSAMS manipulations but we found this  
1077 option to be insufficiently flexible. We will adopt a scripting language capable of handling one or  
1078 several XSAMS data sets, allowing the creation of any simplified projection of XSAMS, unit conversion,  
1079 cross-identification between XSAMS, formatting of the output, handling conditions, loops and data  
1080 structures. The language should be simple enough for general users to learn (e.g. resembling Python  
1081 or other popular programming/scripting languages). The language will be supported by a library of  
1082 critical functions such as automatically analysing XSAMS, unit conversion, etc. This will provide a  
1083 different level of flexibility for end users that could be integrated with asynchronous queries to the  
1084 VAMDC request or with automated sequences of multiple requests.

## 1085 6.5. Prototype of a New Bibliographic Service

1086

1087 We note that all the VAMDC data have a direct reference to the publications where the data have  
1088 been originally presented, described and explained. The idea behind the new bibliographic service we  
1089 have designed and are now prototyping is to use this bibliographic link “in the reverse direction” and  
1090 discover data through publications. The resulting digital library portal, inspired by the *Astrophysics*  
1091 *data system*<sup>70</sup>, provides the community with a unique one-stop shop for the bibliographic information  
1092 contained in VAMDC; the entry point is a tool where users may look for publications. The proposed  
1093 filtering criterion for the search refinement is the author(s), title and year of publication. The results  
1094 corresponding to the submitted bibliographic query are displayed in a tabular form where each line  
1095 corresponds to a publication. For each publication:

- 1096 • VAMDC provides the main bibliographic information complemented by the list of the VAMDC  
1097 nodes containing data related to that particular publication;
- 1098 • when supported by the node, VAMDC provides direct link(s) for extracting the XSAMS data  
1099 related to the publication from the VAMDC node.

1100 This new service may be used as a tool for identifying data-set overlaps between VAMDC nodes.

#### 1101 6.6. Semantic Search of Qualitative Tabular and Graphic Resources in Quantitative Spectroscopy

1102 A semantic search for information resources is possible for systematic data, provided there is  
1103 an explicit description of their properties in the form of ontologies (logical theories) [105]. In the  
1104 Semantic Web approach [186] the rules for constructing such ontologies are defined in the languages  
1105 of their specification [187]. At VAMDC the quality of spectral resources is determined by the data  
1106 standardisation. This includes their analysis, validity control and trust assessment (see Section 5.1).  
1107 A semantic search in molecular spectroscopy was implemented in 2007–2019 to find qualitative  
1108 information resources in quantitative spectroscopy of atmospheric molecules [188], qualitative energy  
1109 levels and molecular transitions<sup>71</sup>[189,190], as well as spectral functions [191], used to solve the  
1110 problems of continuum absorption and to describe the properties of weakly bounded complexes. The  
1111 accumulated experience allowed systematic organisation of the semantic searches for high-quality  
1112 spectral resources, states and transitions, as well as spectral functions in atomic, ionic and solid-state  
1113 spectroscopy that describe the processes of absorption and emission.

1114 A crucial task in the coming years is the organisation of a semantic search for spectral data in  
1115 applied fields (astronomy and atmospheric optics of exoplanets), in which atoms, ions, molecules and  
1116 complexes play an important role. The systematisation of these subjects will simplify the search for  
1117 necessary spectral information. The main challenge that needs to be overcome is the construction of  
1118 a template that allows the user to submit their requirements to be directly implemented as a set of  
1119 queries to a semantic site. For this, it is necessary to build typical ontologies [105] of applied domains.  
1120 The crucial task here is a reduction problem, defining a structure for each of the applications, which  
1121 requires cooperation with experts in these applied domains.

#### 1122 6.7. Visualisation and Data Access from Python

1123 Good data visualisation is important, particularly in data-set exploration. For larger data sets,  
1124 dynamic display becomes essential, wherein the user scrolls through the data and zooms into areas  
1125 of interest. Currently VAMDC provides some static displays of data (generated on the servers as  
1126 web pages) and some dynamic displays (generated by a program on the user’s computer using data  
1127 downloaded from VAMDC). Neither of these approaches works well with large data sets; static pages  
1128 are not sufficient and downloading large and rich data sets to plot only a small fraction of the data is  
1129 frustratingly slow.

---

<sup>70</sup> <https://ui.adsabs.harvard.edu>

<sup>71</sup> <http://wadis.saga.iao.ru/saga2/ontology-3-atomic-molecules/>

1130 Plotting large data sets is a common problem in scientific computing, and in recent years some  
1131 solutions have been developed. The Python libraries Bokeh<sup>72</sup>, Holoviews<sup>73</sup> and Datashader<sup>74</sup> can  
1132 be combined to build plots that can be generated on a server, viewed in a web-browser and that are  
1133 usefully interactive even with large data. The graphics packages also work well in Jupyter notebooks<sup>75</sup>.  
1134 To exploit this, we should provide code that allows such a notebook to extract data from VAMDC,  
1135 either via a downloaded XSAMS-file or directly from data nodes.

#### 1136 6.8. Link Data to Evaluation Ratings

1137 We foresee handling the issue of linking data to evaluation ratings performed by review panels.  
1138 The intention is to facilitate user choices among data sets provided by the various databases. This will  
1139 involve a scientific organisation within VAMDC, collaborations with evaluation bodies and panels  
1140 and, finally, technical developments in order to use the reviewed information.

#### 1141 6.9. Open Science for the Future

1142 VAMDC is collaborating with the [EOSC Secretariat](#) to study an innovative *Flexible Semantic*  
1143 *Mapping Framework* to achieve a scientific and interdisciplinary interoperability between the services  
1144 within the [European Open Science Cloud](#). The VAMDC consortium has explored the development of  
1145 innovative services for automatic data quality assessment based on the interlinking between data and  
1146 scientific papers (see Section 3.2.2) in combination with Artificial Intelligence and semantic techniques.  
1147 In the context of Open Science, this approach may be adopted by any other discipline. The VAMDC  
1148 consortium is evaluating the opportunity to put these ideas into effect as part of a future European  
1149 project proposal.

#### 1150 6.10. Quality Status and Future

1151 It should be stressed that the VAMDC infrastructure does not collectively address the issue of the  
1152 data scientific quality. The scientific quality of the data taken from the e-infrastructure is that of the  
1153 individual databases. The VAMDC infrastructure is currently a technical platform that ensures that  
1154 the exchanged data are compliant with the standards, in particular with the data-format standards.  
1155 As described in Section 5.1 the standardisation imposed quality/coherence checks at the individual  
1156 nodes, and those checks were beneficial to the overall quality of the outputs. The data nodes must be  
1157 compliant with an internal quality chart voted by the board<sup>76</sup>. Some specific quality improvements  
1158 specify that references must be attached to the data, that the transferred data are timestamped and that  
1159 the various queries are stored in the "Query Store" to ensure the tracing of the data. When uncertainties  
1160 are available in the databases, this information is transferred through VAMDC.

1161 In addition, as described above, it is planned to attach external rating reviews to data: rating  
1162 reviews might concern comparison of several sets of data for a single range of applications or might  
1163 concern a single set of data to provide its range of applicability. Obviously we should be aware that  
1164 reviews are only a guide, they depend upon the group of people who performed the review, they can  
1165 rapidly become out of date and should be updated. VAMDC offers an open infrastructure that allows  
1166 third parties to establish some data assessment and to provide such services. VAMDC collects data and  
1167 facilitates the comparison of data from different databases that might contain identical quantities: since  
1168 all VAMDC nodes produce XSAMS formatted output data, it is easy for a user to identify overlaps  
1169 between databases, e.g. by identifying when the same data units have different values.

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72 <https://bokeh.org>

73 <http://holoviews.org>

74 <https://datashader.org>

75 <https://jupyter.org/>

76 <http://www.vamdc.org/structure/how-to-join-us/internal-regulations/>

1170 We would like to stress that VAMDC provides support to the work of scientists, but that users  
1171 should be pro-active with VAMDC to enrich the scientific information. The system and service can be  
1172 steadily improved and augmented by collecting and providing more central statistics about the content  
1173 of the attached databases. Currently the species database allows the display of the species contained in  
1174 the individual databases, but it could additionally list the processes and their range of applicability.  
1175 The bibliographic service will display the papers attached to the data from the different databases, thus  
1176 providing another type of central information system. Additional useful central information would be  
1177 to display what fraction of data content in each database is accessible through VAMDC (sometimes it  
1178 is 100% of data, sometimes it is not).

1179 Finally some users would certainly like to have a "one-stop shop" for their application and such an  
1180 effort can be made by users since VAMDC offers the technical possibility to easily build secondary data  
1181 sets (see the discussion of impact on the BRASS database in Section 5.3.2). The VAMDC infrastructure  
1182 could also provide the means to display such "user oriented secondary data collections" if the users  
1183 wish to make them publicly available. The VAMDC consortium could also be the place where such  
1184 demands are made and then collaborative projects could provide such "user oriented data sets". The  
1185 communities should be aware that the VAMDC effort has already been huge, that the current people  
1186 maintain efficiently the databases and the infrastructure with little manpower and financial resources,  
1187 and that communities must get involved/engaged with VAMDC if they want to ensure the service  
1188 they want.

#### 1189 *6.11. Sustainability*

1190 The above technological and scientific innovations are driving forces for the sustainability of the  
1191 VAMDC e-infrastructure. However, the VAMDC consortium must address the long-term issues of  
1192 renewing the scientific and technical people involved in the curation of atomic and molecular data and  
1193 of maintaining the leadership of these activities at/across institutes and in/across countries.

## 1194 **7. Conclusions**

1195 VAMDC is a sophisticated infrastructure that makes large sets of data publicly available in a  
1196 common format.

1197 A fundamental feature of VAMDC is its ability to connect more databases from atomic and  
1198 molecular domains already described in VAMDC, but also from other domains. Therefore, it serves as  
1199 an ideal platform for sustainability of scientific data.

1200 A crucial key to the evolution of VAMDC is its usage in application software and the involvement  
1201 of users in the orientation of the VAMDC e-infrastructure platform and services. Here, we have  
1202 presented a few user case studies to illustrate this.

1203 A striking point in the evolution of VAMDC is its involvement in data management at the highest  
1204 international level. This places the VAMDC e-infrastructure as an international prototype and example,  
1205 where general concepts are developed and applied, thus providing to the international and national  
1206 communities diverse high-level expertise in data management and handling.

1207 In this paper we have demonstrated once again the strength and coherence of the VAMDC concept  
1208 and the quality and the innovation in the development of the standards and software solutions that  
1209 the VAMDC consortium has delivered. It summarises the advancement of a ten-year effort of a large  
1210 group of leading scientists. The paper has also shown how the VAMDC continues to question the  
1211 current status and to identify current weaknesses, while outlining how it will upgrade its services  
1212 (Sections 4.4 and 6) and make future improvements (see Section 6).

1213 Finally, we provide help to newcomers and to users through detailed documentation and  
1214 tutorials<sup>77</sup>. A 'helpdesk'<sup>78</sup> led by experts in the VAMDC portal and tools answers questions and links  
1215 the user with appropriate organisers of relevant databases as well as supports the inclusion of new  
1216 nodes into VAMDC.

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## 1266 Abbreviations

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<sup>77</sup> <http://www.vamdc.org/activities/research/>

<sup>78</sup> email: support@vamdc.eu

1267 The following abbreviations are used in this manuscript:

1268

A&M	Atomic and Molecular
AGB	Asymptotic Giant Branch
ALMA	Atacama Large Millimeter/submillimeter Array
AMBDAS	Atomic and Molecular Bibliographic Data System
AMDIS	Atomic and Molecular Data Interactive System
API	Application Programming Interface
ASCII	American Standard Code for Information Interchange
ASD	Atomic Spectra Database
ASD-1000	Acetylene Spectroscopic Databank
BASECOL	Rovibrational Collisional Database
BeamDB	Belgrade Electron-Atom/Molecule DataBase
1269 CAS	Chemical Abstracts Service
CASSIS	Centre d'Analyse Scientifique de Spectres Instrumentaux et Synthétiques
CDMS	Cologne Database for Molecular Spectroscopy
CDSD- <i>x</i>	Carbon Dioxide Spectroscopic Databank
CNRS	Centre National de la Recherche Scientifique
CRM	Collisional–Radiative Model
DESIRE	Database on Sixth Row Elements
DOI	Digital Object Identifier
DR	Dielectronic Recombination
DREAM	Database of Rare Earths At Mons University
EII	Electron Impact Ionisation
EOSC	European Open Science Cloud

FAIR	Findable, Accessible, Interoperable, Reusable
FITS	Flexible Image Transport System
GEDE-RDA	Group of European Data Expert in the Research Data Alliance
HAPI	HITRAN Application Programming Interface
HITEMP	High-Temperature Molecular Database
HITRAN	High-resolution Transmission Molecular Absorption Database
HTML	Hypertext Markup Language
IAMDB	Indian Atomic and Molecular DataBase
IDEADB	Innsbruck Dissociative Electron Attachment DataBase
IDP	Interplanetary Dust Particle
INAF	Istituto Nazionale di Astrofisica
InChI	International Chemical Identifier
ISM	Interstellar medium
IP	Iron Project
IPPJ	Institute of Plasma Physics, Nagoya University, Nagoya, Japan
IRAP	Institut de Recherche en Astrophysique et Planétologie
IVOA	International Virtual Observatory Alliance
JIHT RAS	Joint Institute for High Temperatures of the Russian Academy of Sciences
JPL	Jet Propulsion Laboratory
KAERI	Korea Atomic Energy Research Institute
KIDA	KInetic Database for Astrochemistry
LASp	Laboratorio di Astrofisica Sperimentale
LIBS	Laser-Induced Breakdown Spectroscopy
MolLIST	Molecular Line Lists, Intensities and Spectra
NDSD-1000	Nitrogen Dioxide Spectroscopic Databank
NIFS	National Institute for Fusion Science
NIST	National Institute of Standards and Technology
NOEMA	Northern Extended Millimeter Array
NOSD-1000	Nitrous Oxide Spectroscopic Databank
1270 OAC	Osservatorio Astrofisico di Catania
OP	Opacity Project
OVGSO	Observatoire Virtuel du Grand Sud-Ouest
PAH	Polycyclic Aromatic Hydrocarbon
PEARL	Photonic Electronic Atomic Reaction Laboratory
QM	Quantum Mechanics
RADEX	Statistical Equilibrium Radiative Transfer Code
RADMC-3D	Multi-Purpose Radiative Transfer Tool
RDA	Research Data Alliance
RATRAN	Radiative Transfer and Excitation of Molecular Lines Code
RDA	Research Data Alliance
REST	Representational State Transfer
RFNC	Russian Federal Nuclear Centre
SAMP	Simple Application Messaging Protocol
SESAM	Spectroscopy Database Dedicated to Electronic Spectra of Diatomic Molecules
SSHADe	Solid Spectroscopy Hosting Architecture of Databases and Expertise
S&MPO	Spectroscopy and Molecular Properties of Ozone
SSAP	Simple Spectral Access Protocol, an IVOA standard
SQL	Structured Query Language
TAP	Table Access Protocol, an IVOA standard
UDfA	UMIST Database for Astrochemistry
UMIST	University of Manchester Institute of Science and Technology
URL	Uniform Resource Locator
VALD	Vienna Atomic Line Database
VAMDC	Virtual Atomic and Molecular Data Centre
VNIITF	All-Russian Institute of Technical Physics
VO	Virtual Observatory
VSS2	VAMDC SQL Sub-set 2
XSAMS	XML Schema for Atoms, Molecules and Solids

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