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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

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 project¹ 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 project² [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 website³ that provides an access to data and documentation, as well as consortium-related information
32 such as current membership and how to join us⁴.

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 portal⁵ 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 access⁶
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

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

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

^a Paper in preparation ^b (FM, C) ^c (P, C) ^d (P, TC) ^e (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 database⁷ [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, C₂, CH, CO, OH, MgH and SiH. VALD now also
102 provides data for the hyperfine-structure splitting of ⁶Li I, ⁷Li I, ²³Na I, ²⁷Al I, ²⁷Al II, ³⁹K I, ⁴⁰K I, ⁴¹K I,
103 ⁴⁵Sc I, ⁴⁵Sc II, ⁴⁷Ti I, ⁴⁹Ti I, ⁴⁷Ti II, ⁴⁹Ti II, ⁵⁰V I, ⁵¹V I, ⁵¹V II, ⁵⁵Mn I, ⁵⁵Mn II, ⁵⁷Fe I, ⁵⁹Co I, ⁵⁹Co II, ⁶¹Ni I,
104 ⁶³Cu I, ⁶⁵Cu I, ⁶⁷Zn I, ⁶⁷Zn I, ⁶⁹Ga I, ⁶⁹Ga I, ⁷¹Ga I, ⁷¹Ga II, ⁸⁵Rb I, ⁸⁷Rb I, ⁸⁷Sr II, ⁸⁹Y II, ⁹³Nb II, ⁹⁵Mo II,
105 ⁹⁷Mo II, ¹²⁷I I, ¹²⁷I I, ¹³⁵Ba II, ¹³⁷Ba II, ¹³⁹La II, ¹⁴¹Pr I, ¹⁴¹Pr II, ¹⁵¹Eu II, ¹⁵³Eu II, ¹⁵⁵Gd II, ¹⁵⁷Gd II, ¹⁵⁹Tb II,

⁷ <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 project⁸ 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 CHIANTI⁹, 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

⁸ <http://spectr-w3.snz.ru>

⁹ 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 France¹⁰. 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

¹⁰ <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 databases¹¹ 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

¹¹ <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*¹² 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 ¹⁷O and ¹⁸O 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 Reims¹³ and Tomsk¹⁴ 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 website¹⁵. 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

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

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 (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 (C_2H_4 found in Earth's and
290 planetary atmospheres [101]), TFMeCaSDa (CF_4 found in Earth's atmosphere), SHeCaSDa (SF_6 found
291 in Earth's atmosphere), GeCaSDa (GeD_4 found in giant planets' atmospheres) and RuCaSDa (RuO_4
292 important for the nuclear industry).

293 Two new databases have been added recently: TFSiCaSDa [19] concerning the SiF_4 molecule with
294 applications to volcanic gases and UHeCaSDa (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 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 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 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 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"¹⁶ parameters (wavenumber, wavelength, line strength, InChIKey

¹⁶ 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 server¹⁷ where they are presented in the original tabular format.

333 2.1.13. SESAM

334 SESAM¹⁸ 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]¹⁹ 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 Russia²⁰. 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 (KIDA²¹) [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).

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 website²² 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 RADEX²³, RATRAN²⁴ and RADMC-3D²⁵ 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 software²⁶. 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 Observatory²⁷. It has enabled fairly easy access
406 to data (in tabulated and graphical form) of thermally averaged photodissociation cross sections

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/

26 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]. BeamDB²⁸ 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 node²⁹ 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 Italy³⁰ and additional information can be found at its URL³¹. 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.

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, CO₂ and
450 CH₄ 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 online³². The web interface to the relational database, holding the data available through VAMDC,
460 is hosted at the Cagliari Observatory in Italy³³. 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 database³⁴ 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 database³⁵(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

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. SSHADE³⁶ [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 partners³⁷, 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)³⁸ 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 University³⁹. 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 database⁴⁰
527 is described in [38].

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 (IAMDB⁴¹) 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 site⁴², 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.

⁴¹ www.iamdb.org.in

⁴² <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 “(CO₂)(H₂O)”). This will return all datasets
574 with clusters of “(CO₂)_n(H₂O)_m”, ($m, n > 0$). 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-service⁴³ protocol VAMDC-TAP, which is derived from
608 the International Virtual Observatory Alliance (IVOA)⁴⁴ Table Access Protocol (TAP).⁴⁵

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

⁴³ 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.

⁴⁴ <http://ivoa.net/>

⁴⁵ <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)⁴⁶ operates on
612 these virtual tables. The common output format is the XML Schema for Atoms, Molecules and Solids
613 (XSAMS)⁴⁷ [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 registry⁴⁸ 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 portal⁴⁹ [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).

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

Query Execution

Done

Modify query Stop waiting Save query

Comments

Your request

```
select * where ((InchiKey = 'UGFAIRIUMAVXCW-UHFFFAOYSA-N'))
```

Results by node

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. TOPCAT⁵⁰.

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 description⁵¹. 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 database⁵², we provide a versatile
 649 tool to explore the species content of the atomic and molecular VAMDC connected databases. Using
 650 this REST API⁵³ 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.

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

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

⁵² <https://species.vamdc.eu>

⁵³ 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 DOI⁵⁴;
- 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 URL⁵⁵; 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

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

⁵⁵ <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 CH₃Cl 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 CF₄ [162] or NF₃ [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 system⁵⁶ 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.

⁵⁶ <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-package⁵⁷ 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, Django⁵⁸ 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 CASSIS⁵⁹ (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 SSAP⁶⁰ VO or

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 ~ 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 χ^2 minimisation with Jython⁶¹
 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.

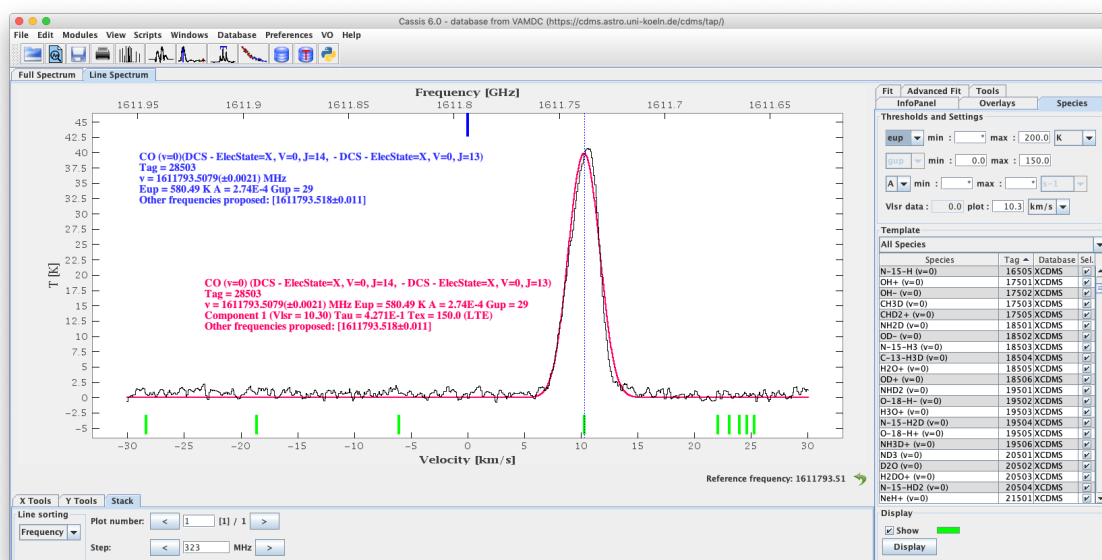


Figure 2. Example of a request made within CASSIS for an observed transition of CO (black) using the CDMS node of VAMDC for the line identification and LTE modelling (red) (see text). The right side of the figure shows the species available in the database and the possible thresholds on the Einstein 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

⁶¹ <https://www.jython.org>

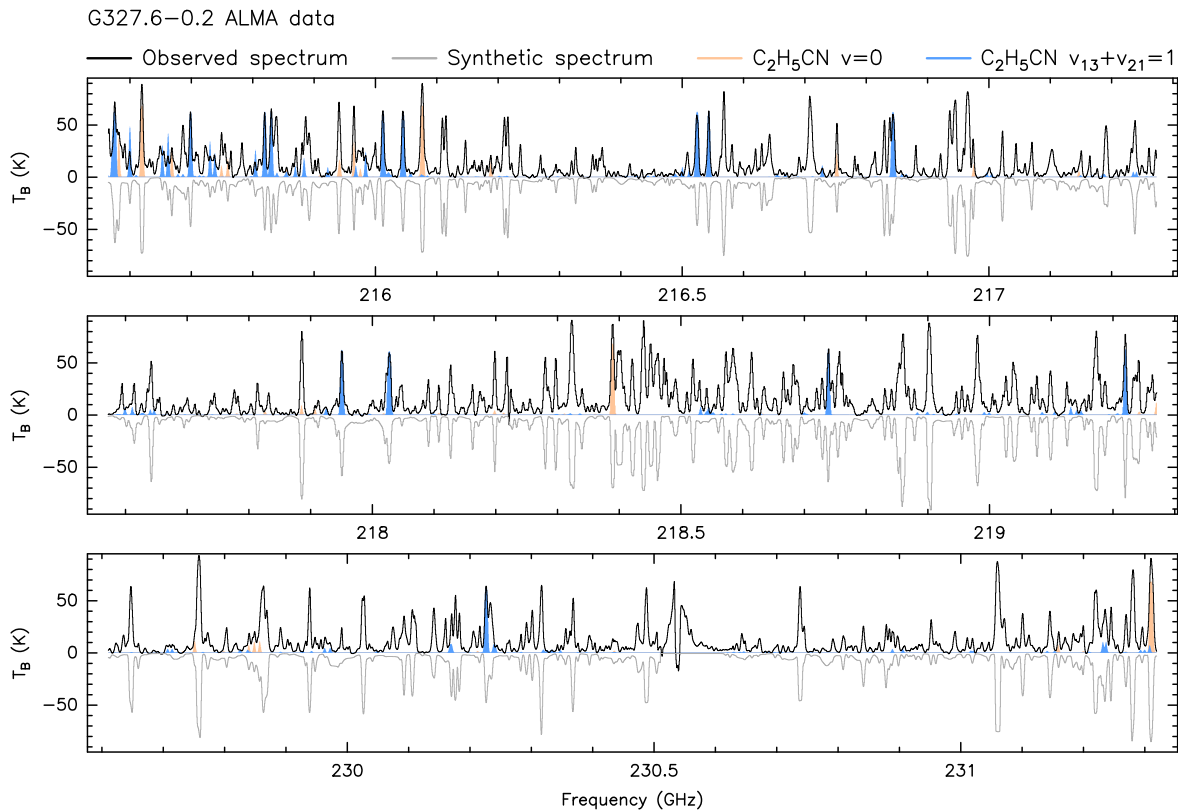


Figure 3. Spectra towards the high-mass star-forming region G327.3-0.6, with the intensity in brightness temperature unit (T_B) observed with the Atacama Large Millimeter/submillimeter Array (ALMA). The myCLASSfit function was used to model the observational data shown in black. Synthetic spectrum including 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 XCLASS⁶² [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 RADEX⁶³ formalism.
 808 Hereby, local overlap of lines can be taken into account as well. Furthermore, non-Gaussian line

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

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

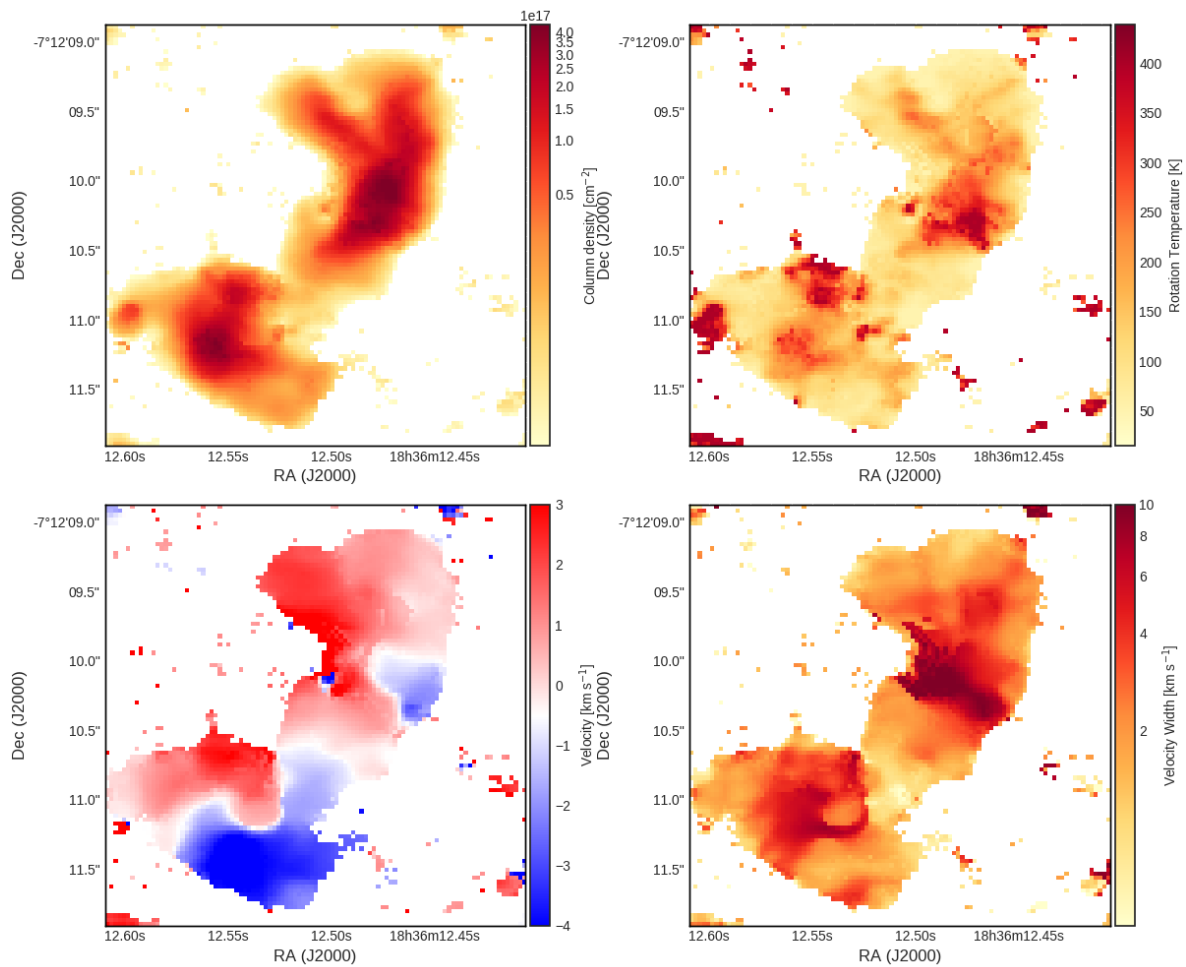


Figure 4. Example of parameter maps created by the myXCLASSMapFit function using nine transitions of CH₃OCHO simultaneously, taken from an ALMA data set of the core of G24.78 [172].

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 stars⁶⁴ [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 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 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;

⁶⁴ 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*⁶⁵ 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).

⁶⁵ 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 URL⁶⁶.

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 portal⁶⁷ 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

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

⁶⁷ <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 standards⁶⁸.

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](#).

⁶⁸ <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"⁶⁹ 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.

⁶⁹ 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*⁷⁰, 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 transitions⁷¹[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.

⁷⁰ <https://ui.adsabs.harvard.edu>

⁷¹ <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 Bokeh⁷², Holoviews⁷³ and Datashader⁷⁴ 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 notebooks⁷⁵.
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 board⁷⁶. 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.

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 tutorials⁷⁷. A 'helpdesk'⁷⁸ 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

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

⁷⁸ 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

1271 **References**

- 1272 1. Dubernet, M.L.; Boudon, V.; Culhane, J.L.; Dimitrijevic, M.S.; Fazliev, A.Z.; Joblin, C.; Kupka, F.; Leto,
1273 G.; Le Sidaner, P.; Loboda, P.A.; Mason, H.E.; Mason, N.J.; Mendoza, C.; Mulas, G.; Millar, T.J.; Nuñez,
1274 L.A.; Perevalov, V.I.; Piskunov, N.; Ralchenko, Y.; Rixon, G.; Rothman, L.S.; Roueff, E.; Ryabchikova, T.A.;
1275 Ryabtsev, A.; Sahal-Bréchet, S.; Schmitt, B.; Schlemmer, S.; Tennyson, J.; Tyuterev, V.G.; Walton, N.A.;
1276 Wakelam, V.; Zeippen, C.J. Virtual atomic and molecular data centre. *J. Quant. Spectrosc. Radiat. Transfer*
1277 **2010**, *111*, 2151–2159. doi:10.1016/j.jqsrt.2010.05.004.
- 1278 2. Zwolf, C.; Dubernet, M.L.; Ba, Y.A.; Moreau, N. Experience and feedbacks from the sustainability for the
1279 virtual atomic and molecular data centre E-infrastructure. IST-Africa Conference Proceedings, 2014, 2014,
1280 pp. 1–9. doi:10.1109/ISTAFRICA.2014.6880621.
- 1281 3. Dubernet, M.L.; Antony, B.; Ba, Y.A.; Babikov, Y.; Bartschat, K.; Boudon, V.; Braams, B.; Chung, H.K.;
1282 Daniel, F.; Delahaye, F.; Del Zanna, G.; de Urquijo, J.; Dimitrijevic, M.; Domaracka, A.; Doronin, M.;
1283 Drouin, B.; Endres, C.; Fazliev, A.; Gagarin, S.; Gordon, I.; Gratier, P.; Heiter, U.; Hill, C.; Jevremovic, D.;
1284 Joblin, C.; Karsprzak, A.; Krishnakumar, E.; Leto, G.; Loboda, P.A.; Louge, T.; Maclot, S.; Marinkovic,
1285 B.; Markwick Kemper, A.; Marquart, T.; Mason, H.; Mason, N.; Mendoza, C.; Mihajlov, A.; Millar, T.;
1286 Moreau, N.; Mulas, G.; Pakhomov, Y.; Palmeri, P.; Pancheshnyi, S.; Perevalov, V.I.; Piskunov, N.; Postler,
1287 J.; Quinet, Pascal and Quintas Sánchez, E.L.; Ralchenko, Y.; Rhee, Y.J.; Rixon, G.; Rothman, L.; Roueff,
1288 E.; Ryabchikova, T.; Sahal-Brechet, S.; Scheier, P.; Schlemmer, S.; Schmitt, B.; Stempels, E.; Tashkun, S.;
1289 Tennyson, J.; Tyuterev, V.; Vujcic, V.; Wakelam, V.; Walton, N.; Zatsarinny, O.; Zeippen, C.; Zwölf, C.M. The
1290 Virtual Atomic and Molecular Data Centre (VAMDC) Consortium. *Journal of Physics B: Atomic, Molecular*
1291 *and Optical Physics* **2016**, *49*, 074003. doi:10.1088/0953-4075/49/7/074003.
- 1292 4. Emoto, M.; Murakami, I.; Kato, D.; Yoshida, M.; Kato, M.; Imazu, S. Improvement of the NIFS Atom and
1293 Molecular Database. *Atoms* **2019**, *7*, 91. doi:10.3390/atoms7030091.
- 1294 5. Murakami, I.; Kato, D.; Kato, M.; Sakaue, H.A. Atomic and molecular database and data evaluation
1295 activities at the National Institute for Fusion Science. *Fusion Sci. Technol.* **2013**, *63*, 400–405.
1296 doi:10.13182/FST13-A16448.
- 1297 6. Ryabchikova, T.; Piskunov, N.; Kurucz, R.L.; Stempels, H.C.; Heiter, U.; Pakhomov, Y.; Barklem, P.S. A major
1298 upgrade of the VALD database. *Physica Scripta* **2015**, *90*, 054005. doi:10.1088/0031-8949/90/5/054005.
- 1299 7. Kramida, A.; Yu. Ralchenko.; Reader, J.; and NIST ASD Team. NIST Atomic Spectra Database (ver. 5.7.1),
1300 [Online]. Available: <https://physics.nist.gov/asd> [2020, July 9]. National Institute of Standards and
1301 Technology, Gaithersburg, MD., 2019.
- 1302 8. Skobelev, I.Y.; Loboda, P.A.; Gagarin, S.V.; Ivliev, S.V.; Kozlov, A.I.; Morozov, S.V.; S. A. Pikuz, J.; Pikuz,
1303 T.A.; Popova, V.V.; Faenov, A.Y. The Spectr-W³ Database on the Spectroscopic Properties of Atoms and
1304 Ions. *Optics and Spectroscopy* **2016**, *120*, 507–514.
- 1305 9. Del Zanna, G.; Young, P.R. Atomic data for plasma spectroscopy: the CHIANTI database, improvements
1306 and challenges. *Submitted to Atoms* **2020**.
- 1307 10. Hummer, D.G.; Berrington, K.A.; Eissner, W.; Pradhan, A.K.; Saraph, H.E.; Tully, J.A. Atomic data from
1308 the IRON project. I. Goals and methods. *A&A* **1993**, *279*, 298–309.
- 1309 11. Cunto, W.; Mendoza, C.; Ochsenbein, F.; Zeippen, C.J. TOPbase at the CDS. *A&A* **1993**, *275*, L5–L8.
- 1310 12. Sahal-Bréchet, S.; Dimitrijević, M.S.; Moreau, N. Virtual Laboratory Astrophysics and the Stark-B database
1311 VAMDC node: A resource for electron and ion impact widths and shifts of isolated lines. *Journal of Physics:*
1312 *Conference Series* **2020**, *1412*, 132052.
- 1313 13. Roueff, E.L.; Sahal-Bréchet, S.; M., D.; Moreau, N.; Abgrall, H. The spectroscopic atomic and molecular
1314 databases at Paris Observatory. *Atoms* **2020**, *8*, 36–48.
- 1315 14. Endres, C.P.; Schlemmer, S.; Schilke, P.; Stutzki, J.; Mueller, H.S.P. The Cologne Database for Molecular
1316 Spectroscopy, CDMS, in the Virtual Atomic and Molecular Data Centre, VAMDC. *J. Mol. Spect.* **2016**,
1317 *327*, 95–104.
- 1318 15. Pickett, H.M.; Poynter, R.L.; Cohen, E.A.; Delitsky, M.L.; Pearson, J.C.; Müller, H.S.P. Submillimeter,
1319 millimeter and microwave spectral line catalog. *J. Quant. Spectrosc. Radiat. Transfer* **1998**, *60*, 883–890.
1320 doi:10.1016/S0022-4073(98)00091-0.
- 1321 16. Gordon, I.E.; Rothman, L.S.; Hill, C.; Kochanov, R.V.; Tan, Y.; Bernath, P.F.; Birk, M.; Boudon, V.; Campargue,
1322 A.; Chance, K.V.; Drouin, B.J.; Flaud, J.M.; Gamache, R.R.; Hodges, J.T.; Jacquemart, D.; Perevalov, V.I.;

- 1323 Perrin, A.; Shine, K.P.; Smith, M.A.H.; Tennyson, J.; Toon, G.C.; Tran, H.; Tyuterev, V.G.; Barbe, A.; Császár,
1324 A.G.; Devi, V.M.; Furtenbacher, T.; Harrison, J.J.; Hartmann, J.M.; Jolly, A.; Johnson, T.J.; Karman, T.;
1325 Kleiner, I.; Kyuberis, A.A.; Loos, J.; Lyulin, O.M.; Massie, S.T.; Mikhailenko, S.N.; Moazzen-Ahmadi, N.;
1326 Müller, H.S.P.; Naumenko, O.V.; Nikitin, A.V.; Polyansky, O.L.; Rey, M.; Rotger, M.; Sharpe, S.W.; Sung,
1327 K.; Starikova, E.; Tashkun, S.A.; Vander Auwera, J.; Wagner, G.; Wilzewski, J.; Wcisło, P.; Yu, S.; Zak, E.J.
1328 The *HITRAN* 2016 molecular spectroscopic database. *J. Quant. Spectrosc. Radiat. Transfer* **2017**, *203*, 3–69.
1329 doi:10.1016/j.jqsrt.2017.06.038.
- 1330 17. Babikov, Y.; Mikhailenko, S.; Barbe, A.; Tyuterev, V. S&MPO - An information system for ozone spectroscopy
1331 on the WEB. *J. Quant. Spectrosc. Radiat. Transfer* **2014**, *145*, 169–196. doi:10.1016/j.jqsrt.2014.04.024.
- 1332 18. Richard, C.; Boudon, V.; Rotger, M. Calculated spectroscopic databases for the VAMDC portal: New
1333 molecules and improvements. *J. Quant. Spectrosc. Radiat Transfer* **2020**, *251*, 107096–1–107096–13.
- 1334 19. Boudon, V.; Manceron, L.; Richard, C. High-resolution spectroscopy and analysis of the ν_3 , ν_4 and $2\nu_4$ bands
1335 of SiF₄ in natural isotopic abundance. *J. Quant. Spectrosc. Radiat Transfer* **2020**, *253*, 107114–1–107114–20.
- 1336 20. Tashkun, S.A.; Perevalov, V.I.; Gamache, R.R.; Lamouroux, J. CDS-296, high-resolution carbon
1337 dioxide spectroscopic databank: An update. *J. Quant. Spectrosc. Radiat. Transfer* **2019**, *228*, 124–131.
1338 doi:10.1016/j.jqsrt.2019.03.001.
- 1339 21. Tashkun, S.A.; Perevalov, V.I. CDS-4000: High-resolution, high-temperature carbon dioxide spectroscopic
1340 databank. *J. Quant. Spectrosc. Radiat. Transfer* **2011**, *112*, 1403–1410. doi:10.1016/j.jqsrt.2011.03.005.
- 1341 22. Tashkun, S.A.; Perevalov, V.I.; Lavrentieva, N.N. NOSD-1000, the high-temperature nitrous oxide
1342 spectroscopic databank. *J. Quant. Spectrosc. Radiat. Transfer* **2016**, *177*, 43–48. doi:10.1016/j.jqsrt.2015.11.014.
- 1343 23. Lukashetskaya, A.A.; Lavrentieva, N.N.; Dudaryonok, A.C.; Perevalov, V.I. NDS-1000: High-resolution,
1344 high-temperature Nitrogen Dioxide Spectroscopic Databank. *J. Quant. Spectrosc. Radiat. Transfer* **2016**,
1345 *184*, 205–217. doi:10.1016/j.jqsrt.2016.07.014.
- 1346 24. Lyulin, O.M.; Perevalov, V.I. ASD-1000: High-resolution, high-temperature acetylene spectroscopic
1347 databank. *J. Quant. Spectrosc. Radiat. Transfer* **2017**, *201*, 94–103. doi:10.1016/j.jqsrt.2017.06.032.
- 1348 25. Akhlyostin, A.; Apanovich, Z.; Fazliev, A.; Kozodoev, A.; Lavrentiev, N.; Privezentsev, A.; Rodimova,
1349 O.; Voronina, S.; Császár, A.; Tennyson, J. The current status of the W@DIS information
1350 system. 22-nd International Symposium Atmospheric and Ocean Optics: Atmospheric Physics, 2016.
1351 doi:10.1117/12.2249235.
- 1352 26. Wakelam, V.; Herbst, E.; Loison, J.C.; Smith, I.W.M.; Chandrasekaran, V.; Pavone, B.; Adams, N.G.;
1353 Bacchus-Montabonel, M.C.; Bergeat, A.; Béroff, K.; Bierbaum, V.M.; Chabot, M.; Dalgarno, A.; van
1354 Dishoeck, E.F.; Faure, A.; Geppert, W.D.; Gerlich, D.; Galli, D.; Hébrard, E.; Hersant, F.; Hickson, K.M.;
1355 Honvault, P.; Klippenstein, S.J.; Le Picard, S.; Nyman, G.; Pernot, P.; Schlemmer, S.; Selsis, F.; Sims, I.R.;
1356 Talbi, D.; Tennyson, J.; Troe, J.; Wester, R.; Wiesenfeld, L. A Kinetic Database for Astrochemistry (KIDA).
1357 *Astrophys. J. Suppl.* **2012**, *199*, 21, [1201.5887]. doi:10.1088/0067-0049/199/1/21.
- 1358 27. Wakelam, V.; Loison, J.C.; Herbst, E.; Pavone, B.; Bergeat, A.; Béroff, K.; Chabot, M.; Faure, A.; Galli,
1359 D.; Geppert, W.D.; Gerlich, D.; Gratier, P.; Harada, N.; Hickson, K.M.; Honvault, P.; Klippenstein, S.J.;
1360 Le Picard, S.D.; Nyman, G.; Ruaud, M.; Schlemmer, S.; Sims, I.R.; Talbi, D.; Tennyson, J.; Wester, R.
1361 The 2014 KIDA Network for Interstellar Chemistry. *Astrophys. J. Suppl.* **2015**, *217*, 20, [1503.01594].
1362 doi:10.1088/0067-0049/217/2/20.
- 1363 28. McElroy, D.; Walsh, C.; Markwick, A.J.; Cordiner, M.A.; Smith, K.; Millar, T.J. The
1364 UMIST database for astrochemistry 2012. *A&A* **2013**, *550*, A36, [arXiv:astro-ph.SR/1212.6362].
1365 doi:10.1051/0004-6361/201220465.
- 1366 29. Dubernet, M.L.; Alexander, M.H.; Ba, Y.A.; Balakrishnan, N.; Balança, C.; Ceccarelli, C.; Cernicharo, J.;
1367 Daniel, F.; Dayou, F.; Doronin, M.; Dumouchel, F.; Faure, A.; Feautrier, N.; Flower, D.R.; Grosjean, A.;
1368 Halvick, P.; Klos, J.; Lique, F.; McBane, G.C.; Marinakis, S.; Moreau, N.; Moszynski, R.; Neufeld, D.A.;
1369 Roueff, E.; Schilke, P.; Spielfiedel, A.; Stancil, P.C.; Stoecklin, T.; Tennyson, J.; Yang, B.; Vasserot, A.M.;
1370 Wiesenfeld, L. BASECOL2012: A collisional database repository and web service within the Virtual Atomic
1371 and Molecular Data Centre (VAMDC). *A&A* **2013**, *553*, A50. doi:10.1051/0004-6361/201220630.
- 1372 30. Ba, Y.; Dubernet, M.; Moreau, N.; Zwolf, C. BASECOL (basecol.vamdc.org) new technical design. *Submitted*
1373 *to Atoms* **2020**.

- 1374 31. Vujčić, V.; Jevremović, D.; Mihajlov, A.; Ignjatović, L.M.; Srećković, V.; Dimitrijević, M.; Malović, M. MOL-D:
1375 A Collisional Database and Web Service within the Virtual Atomic and Molecular Data Center. *J. Astrophys.*
1376 *Astron.* **2015**, *36*, 0.
- 1377 32. Jevremović, D.; Srećković, V.A.; Marinković, B.P.; Vujčić, V. Databases for collisional and radiative processes
1378 in small molecules needed for spectroscopy use in astrophysics. *Contrib. Astron. Obs. Skalnate Pleso* **2020**,
1379 *50*, 44–54.
- 1380 33. Marinković, B.P.; Vujčić, V.; Sushko, G.; Vudragović, D.; Marinković, D.B.; Đorđević, S.; Ivanović, S.; Nešić,
1381 M.; Jevremović, D.; Solov'ov, A.V.; Mason, N.J. Development of collisional data base for elementary
1382 processes of electron scattering by atoms and molecules. *Nuclear Instruments and Methods in Physics Research*
1383 *Section B: Beam Interactions with Materials and Atoms* **2015**, *354*, 90 – 95. 26th International Conference on
1384 Atomic Collisions in Solids, doi:<https://doi.org/10.1016/j.nimb.2014.12.039>.
- 1385 34. Gorfinkiel, J.D.; Ptasincka, S. Electron scattering from molecules and molecular aggregates of
1386 biological relevance. *Journal of Physics B: Atomic, Molecular and Optical Physics* **2017**, *50*, 182001.
1387 doi:10.1088/1361-6455/aa8572.
- 1388 35. Schmitt, B.; Bollard, P.; Damien, A.; Garenne, A.; Bonal, L.; Gorbacheva, M.; the SSHADE partner's
1389 consortium. SSHADE: Solid Spectroscopy Hosting Architecture of Databases and Expertise and its
1390 databases. online, 2018. database Infrastructure, publisher: OSUG Data Center, <https://www.sshade.eu>,
1391 doi:10.26302/SSHADE.
- 1392 36. Mallocci, G.; Joblin, C.; Mulas, G. On-line database of the spectral properties of polycyclic
1393 aromatic hydrocarbons. *Chem. Phys.* **2007**, *332*, 353–359, [[arXiv:astro-ph/0701254](https://arxiv.org/abs/astro-ph/0701254)].
1394 doi:10.1016/j.chemphys.2007.01.001.
- 1395 37. Chubb, K.L.; Rocchetto, M.; Yurchenko, S.N.; Min, M.; Waldmann, I.; Barstow, J.K.; Molliere, P.; Al-Refaiie,
1396 A.F.; Phillips, M.; Tennyson, J. The ExoMolOP Database: Cross-sections and K-tables for Molecules of
1397 Interest in High-Temperature Exoplanet Atmospheres. *A&A* **2020**.
- 1398 38. Fivet, V.; Quinet, P.; Palmeri, P.; Biémont, E.; Xu, H. Transition probabilities and lifetimes for atoms and
1399 ions from the sixth row of the periodic table and the database DESIRE. *J. Electr. Spectrosc. Rel. Phen.* **2007**,
1400 *250*, 156–158.
- 1401 39. Quinet, P.; Palmeri, P. Current status and developments of the Atomic Database on Rare-Earths at Mons
1402 University (DREAM). *Atoms* **2020**, *8*, 18.
- 1403 40. Kwon, D.H.; K.-B. Chai.; and KAERI Atomic Data Center Team. Photonic Electronic Atomic Reaction
1404 Laboratory database, [Online]. Available: <http://pearl.kaeri.re.kr>.
- 1405 41. Takayanagi, K.; Suzuki, H. Cross sections for Atomic Processes Vol.1. Processes Involving Hydrogen
1406 Isotopes, Their Ions, Electrons and Photons. Technical Report IPPJ-DT-48, Institute of Plasma Physics,
1407 Nagoya University, Nagoya, Japan, 1975.
- 1408 42. Takayanagi, K.; Suzuki, H. Cross sections for Atomic Processes Vol.2. Processes Involving Hydrogen and
1409 Helium Isotopes, Their Ions, Electrons and Photons. Technical Report IPPJ-DT-50, Institute of Plasma
1410 Physics, Nagoya University, Nagoya, Japan, 1976.
- 1411 43. Kato, T.; Itikawa, Y.; Kanada, Y.; Watanabe, R. Database and Retrieval-Display System of Atomic Data for
1412 Fusion. *Physica Scripta* **1981**, *23*, 198–201. doi:10.1088/0031-8949/23/2/027.
- 1413 44. Murakami, I.; Kato, M.; Emoto, M.; Kato, D.; Sakaue, H.A.; Kawate, T. NIFS Atomic and Molecular
1414 Database for collision processes. *submitted to Atoms* **2020**.
- 1415 45. Biémont, E.; Palmeri, P.; Quinet, P. A New Database of Astrophysical Interest. *Astrophys. Space Sci.* **1999**,
1416 *269*, 635–637. doi:10.1023/A:1017049314691.
- 1417 46. Pakhomov, Y.V.; Ryabchikova, T.A.; Piskunov, N.E. Hyperfine Splitting in the VALD Database of
1418 Spectral-line Parameters. *Astronomy Reports* **2019**, *63*, 1010–1021, [[arXiv:astro-ph/1911.03189](https://arxiv.org/abs/astro-ph/1911.03189)].
1419 doi:10.1134/S1063772919120047.
- 1420 47. Ryabchikova, T.; Piskunov, N.; Sitnova, T. Evaluation of the Recent Atomic Data for Fe uc(i) Lines Based
1421 on Solar and Stellar Spectra. *Solar Physics* **2019**, *294*, 156. doi:10.1007/s11207-019-1543-2.
- 1422 48. Pakhomov, Y.V.; Ryabchikova, T.A. Evolution of spectral line parameters database VALD. *INASAN Science*
1423 *Reports* **2019**, *4*, 79–84. doi:10.26087/INASAN.2019.4.2.014.
- 1424 49. Ryabchikova, T.; Pakhomov, Y.; Piskunov, N. VALD: The Meeting Point of Data Producers and Data Users.
1425 *Galaxies* **2018**, *5*, 93. doi:10.3390/galaxies6030093.

- 1426 50. Pakhomov, Y.V.; Ryabchikova, T.A. Virtual atomic and molecular data centre VAMDC. *Stars and Satellites*,
1427 Proceedings of the Memorial Conference Devoted to A.G. Masevich 100th Anniversary; Shustov, B.M.;
1428 Wiebe, D.S., Eds., 2018, pp. 402–408. doi:10.26087/INASAN.2018.2.2.065.
- 1429 51. Pakhomov, Y.V. Method of spectral wavelength calibration using the VALD database. *Stars and Satellites*,
1430 Proceedings of the Memorial Conference Devoted to A.G. Masevich 100th Anniversary; Shustov, B.M.;
1431 Wiebe, D.S., Eds., 2018, pp. 374–379. doi:10.26087/INASAN.2018.2.2.060.
- 1432 52. Pakhomov, Y.; Piskunov, N.; Ryabchikova, T. VALD3: Current Developments. *Stars: From Collapse to*
1433 *Collapse*; Balega, Y.Y.; Kudryavtsev, D.O.; Romanyuk, I.I.; Yakunin, I.A., Eds., 2017, Vol. 510, *Astronomical*
1434 *Society of the Pacific Conference Series*, p. 518, [arXiv:astro-ph.IM/1710.10854].
- 1435 53. Kramida, A. NIST Atomic Spectroscopy Bibliographic Databases, [Online]. Available: URL
1436 <https://www.nist.gov/pml/nist-atomic-spectra-bibliographic-databases> [2020, July 9]. National
1437 Institute of Standards and Technology, Gaithersburg, MD., 2019.
- 1438 54. Kramida, A.; Olsen, K.; Yu, Ralchenko. NIST LIBS Database, [Online]. Available:
1439 <https://physics.nist.gov/PhysRefData/ASD/LIBS/lib-form.html> [2020, July 9]. National Institute
1440 of Standards and Technology, Gaithersburg, MD., 2019.
- 1441 55. Dere, K.P.; Landi, E.; Mason, H.E.; Monsignori Fossi, B.C.; Young, P.R. CHIANTI - an atomic database for
1442 emission lines. *Astrophys. J. Suppl.* **1997**, *125*, 149.
- 1443 56. Del Zanna, G.; Dere, K.P.; Young, P.R.; Landi, E.; Mason, H.E. CHIANTI - An atomic database for emission
1444 lines. Version 8. *A&A* **2015**, *582*, A56. doi:10.1051/0004-6361/201526827.
- 1445 57. Dere, K.P.; Del Zanna, G.; Young, P.R.; Landi, E.; Sutherland, R.S. CHIANTI—An Atomic Database for
1446 Emission Lines. XV. Version 9, Improvements for the X-Ray Satellite Lines. *Astrophys. J. Suppl.* **2019**, *241*, 22.
1447 doi:10.3847/1538-4365/ab05cf.
- 1448 58. Seaton, M.J. Atomic data for opacity calculations. I. General description. *J. of Phys. B Atom. Molec. Phys.*
1449 **1987**, *20*, 6363–6378. doi:10.1088/0022-3700/20/23/026.
- 1450 59. Cunto, W.; Mendoza, C. The Opacity Project - the Topbase Atomic Database. *Revista Mexicana de Astronomía*
1451 *y Astrofísica* **1992**, *23*, 107.
- 1452 60. Berrington, K.A.; Eissner, W.B.; Norrington, P.H. RMATRIX1: Belfast atomic R-matrix codes. *Computer*
1453 *Physics Communications* **1995**, *92*, 290–420.
- 1454 61. Ballance, C.P.; Griffin, D.G. Relativistic radiatively damped R-matrix calculation of the electron-impact
1455 excitation of W46+. *J. Phys. B* **2006**, *39*, 3617. doi:10.1088/0953-4075/39/17/017.
- 1456 62. Badnell, N.R. A Breit-Pauli distorted wave implementation for AUTOSTRUCTURE. *Computer Physics*
1457 *Communications* **2011**, *182*, 1528–1535.
- 1458 63. Badnell, N.R.; Bautista, M.A.; Butler, K.; Delahaye, F.; Mendoza, C.; Palmeri, P.; Zeippen, C.J.; Seaton,
1459 M.J. Updated opacities from the Opacity Project. *M. N. R. A. S.* **2005**, *360*, 458–464, [astro-ph/0410744].
1460 doi:10.1111/j.1365-2966.2005.08991.x.
- 1461 64. Delahaye, F.; Zwölf, C.M.; Zeippen, C.J.; Mendoza, C. IPOPv2 online service for the generation of
1462 opacity tables. *J. Quant. Spectrosc. Radiat. Transfer* **2016**, *171*, 66–72, [arXiv:astro-ph.SR/1511.07260].
1463 doi:10.1016/j.jqsrt.2015.11.010.
- 1464 65. Sahal-Bréchet, S.; Dimitrijević, M.S.; Moreau, N.; Ben Nessib, N. The Stark-B Database as a Resource for
1465 “Stark” Widths and Shifts Data: State of Advancement and Program of Development. *Advances in Space*
1466 *Research* **2014**, *54*, 1148–1151.
- 1467 66. Sahal-Bréchet, S.; Dimitrijević, M.S.; Moreau, N.; Ben Nessib, N. The Stark-B Database VAMDC node:
1468 a Repository for Spectral Line Broadening and Shifts Due to Collisions with Charged Particles. *Physica*
1469 *Scripta* **2015**, *50*, 054008.
- 1470 67. Dimitrijević, M.S.; Sahal-Bréchet, S.; Moreau, N. The Stark-B Database, A Node of Virtual Atomic and
1471 Molecular Data Center (VAMDC). *Publications of the Astronomical Observatory of Belgrade* **2018**, *98*, 285–288.
- 1472 68. Sahal-Bréchet, S.; Dimitrijević, M.S.; Ben Nessib, N. Widths and Shifts of Isolated Lines of Neutral and Ionized
1473 Atoms Perturbed by Collisions With Electrons and Ions: An Outline of the Semiclassical Perturbation (SCP)
1474 Method and of the Approximations Used for the Calculations. *Atoms* **2014**, *2*, 225–252.
- 1475 69. Dimitrijević, M.S.; Konjević, N. Stark broadening of doubly and triply ionized atoms. *J. Quant. Spectrosc.*
1476 *Radiat. Transfer* **1980**, *24*, 451–459.
- 1477 70. Sahal-Bréchet, S.; Dimitrijević, M.S.; Ben Nessib, N. Comparisons and comments on electron and ion
1478 impact profiles of spectral lines. *Baltic Astronomy* **2011**, *20*, 523–530.

- 1479 71. Pearson, J.C.; Mueller, H.S.P.; Pickett, H.M.; Cohen, E.A.; Drouin, B.J. Introduction to submillimeter,
1480 millimeter and microwave spectral line catalog. *J. Quant. Spectrosc. Radiat. Transfer* **2010**, *111*, 1614–1616.
1481 doi:10.1016/j.jqsrt.2010.02.002}.
- 1482 72. Endres, C.; Schlemmer, S.; Drouin, B.; Pearson, J.; Müller, H.S.P.; Schilke, P.; Stutzki, J. Improved
1483 Infrastructure for CdmS and JPL Molecular Spectroscopy Catalogues. 69th International Symposium on
1484 Molecular Spectroscopy, 2014.
- 1485 73. Müller, H.S.P.; Thorwirth, S.; Roth, D.A.; Winnewisser, G. The Cologne Database for Molecular
1486 Spectroscopy, CDMS. *A&A* **2001**, *370*, L49–L52. doi:10.1051/0004-6361:20010367.
- 1487 74. Müller, H.S.P.; Schlöder, F.; Stutzki, J.; Winnewisser, G. The Cologne Database for Molecular Spectroscopy,
1488 CDMS: a useful tool for astronomers and spectroscopists. *Journal of Molecular Structure* **2005**, *742*, 215–227.
1489 doi:10.1016/j.molstruc.2005.01.027.
- 1490 75. McClatchey, R.; Benedict, W.; Clough, S.; Burch, D.; Calfee, R.; Fox, K.; Rothman, L.; Garing, J. AFCRL
1491 Atmospheric Absorption Line Parameters Compilation. Technical Report 434, Optical Physics Laboratory,
1492 1973.
- 1493 76. Rothman, L.S. Atmospheric absorption-line parameters: the HITRAN data base (A). *Journal of the Optical*
1494 *Society of America (1917-1983)* **1983**, *73*.
- 1495 77. Rothman, L.S.; Gamache, R.R.; Goldman, A.; Brown, L.R.; Toth, R.A.; Pickett, H.M.; Poynter, R.L.; Flaud,
1496 J.M.; Camy-Peyret, C.; Barbe, A.; Husson, N.; Rinsland, C.P.; Smith, M.A.H. The HITRAN database: 1986
1497 edition. *Applied Optics* **1987**, *26*, 4058. doi:10.1364/AO.26.004058.
- 1498 78. Rothman, L.; Gamache, R.; Tipping, R.; Rinsland, C.; Smith, M.; Benner, D.; Devi, V.; Flaud, J.M.;
1499 Camy-Peyret, C.; Perrin, A.; Goldman, A.; Massie, S.; Brown, L.; Toth, R. The HITRAN molecular
1500 database: Editions of 1991 and 1992. *Journal of Quantitative Spectroscopy and Radiative Transfer* **1992**,
1501 *48*, 469–507. doi:10.1016/0022-4073(92)90115-K.
- 1502 79. Rothman, L.; Rinsland, C.; Goldman, A.; Massie, S.T.; D.P., E.; Flaud, J.M.; Perrin, A.; Camy-Peyret, C.;
1503 Dana, V.; Mandin, J.; J., S.; McCann, A.; Gamache, R.; Wattson, R.; Yoshino, K.; Chance, K.; Jucks, K.; Brown,
1504 L.; Nemtchinov, V.; Varanasi, P. The HITRAN Molecular Spectroscopic Database and HAWKS (HITRAN
1505 Atmospheric Workstation): 1996 Edition. *Journal of Quantitative Spectroscopy and Radiative Transfer* **1998**,
1506 *60*, 665–710. doi:10.1016/S0022-4073(98)00078-8.
- 1507 80. Rothman, L.; Barbe, A.; Chris Benner, D.; Brown, L.; Camy-Peyret, C.; Carleer, M.; Chance, K.; Clerbaux,
1508 C.; Dana, V.; Devi, V.; Fayt, A.; Flaud, J.M.; Gamache, R.; Goldman, A.; Jacquemart, D.; Jucks, K.; Lafferty,
1509 W.; Mandin, J.Y.; Massie, S.; Nemtchinov, V.; Newnham, D.; Perrin, A.; Rinsland, C.; Schroeder, J.; Smith,
1510 K.; Smith, M.; Tang, K.; Toth, R.; Vander Auwera, J.; Varanasi, P.; Yoshino, K. The HITRAN molecular
1511 spectroscopic database: edition of 2000 including updates through 2001. *Journal of Quantitative Spectroscopy*
1512 *and Radiative Transfer* **2003**, *82*, 5–44. doi:10.1016/S0022-4073(03)00146-8.
- 1513 81. Rothman, L.; Jacquemart, D.; Barbe, A.; Chris Benner, D.; Birk, M.; Brown, L.; Carleer, M.; Chackerian,
1514 C.; Chance, K.; Coudert, L.; Dana, V.; Devi, V.; Flaud, J.M.; Gamache, R.; Goldman, A.; Hartmann, J.M.;
1515 Jucks, K.; Maki, A.; Mandin, J.Y.; Massie, S.; Orphal, J.; Perrin, A.; Rinsland, C.; Smith, M.; Tennyson,
1516 J.; Tolchenov, R.; Toth, R.; Vander Auwera, J.; Varanasi, P.; Wagner, G. The HITRAN 2004 molecular
1517 spectroscopic database. *Journal of Quantitative Spectroscopy and Radiative Transfer* **2005**, *96*, 139–204.
1518 doi:10.1016/j.jqsrt.2004.10.008.
- 1519 82. Rothman, L.S.; Gordon, I.E.; Barbe, A.; Benner, D.C.; Bernath, P.F.; Birk, M.; Boudon, V.; Brown, L.R.;
1520 Campargue, A.; Champion, J.P.; Chance, K.; Coudert, L.H.; Dana, V.; Devi, V.M.; Fally, S.; Flaud, J.M.;
1521 Gamache, R.R.; Goldman, A.; Jacquemart, D.; Kleiner, I.; Lacombe, N.; Lafferty, W.J.; Mandin, J.Y.;
1522 Massie, S.T.; Mikhailenko, S.N.; Miller, C.E.; Moazzen-Ahmadi, N.; Naumenko, O.V.; Nikitin, A.V.;
1523 Orphal, J.; Perevalov, V.I.; Perrin, A.; Predoi-Cross, A.; Rinsland, C.P.; Rotger, M.; Šimečková, M.; Smith,
1524 M.A.H.; Sung, K.; Tashkun, S.A.; Tennyson, J.; Toth, R.A.; Vandaele, A.C.; Vander Auwera, J. The
1525 HITRAN 2008 molecular spectroscopic database. *J. Quant. Spectrosc. Radiat. Transfer* **2009**, *110*, 533–572.
1526 doi:10.1016/j.jqsrt.2009.02.013.
- 1527 83. Rothman, L.S.; Gordon, I.E.; Babikov, Y.; Barbe, A.; Chris Benner, D.; Bernath, P.F.; Birk, M.; Bizzocchi,
1528 L.; Boudon, V.; Brown, L.R.; Campargue, A.; Chance, K.; Cohen, E.A.; Coudert, L.H.; Devi, V.M.; Drouin,
1529 B.J.; Fayt, A.; Flaud, J.M.; Gamache, R.R.; Harrison, J.J.; Hartmann, J.M.; Hill, C.; Hodges, J.T.; Jacquemart,
1530 D.; Jolly, A.; Lamouroux, J.; Le Roy, R.J.; Li, G.; Long, D.A.; Lyulin, O.M.; Mackie, C.J.; Massie, S.T.;
1531 Mikhailenko, S.; Müller, H.S.P.; Naumenko, O.V.; Nikitin, A.V.; Orphal, J.; Perevalov, V.; Perrin, A.;

- 1532 Polovtseva, E.R.; Richard, C.; Smith, M.A.H.; Starikova, E.; Sung, K.; Tashkun, S.; Tennyson, J.; Toon, G.C.;
1533 Tyuterev, V.G.; Wagner, G. The HITRAN2012 molecular spectroscopic database. *J. Quant. Spectrosc. Radiat.*
1534 *Transfer* **2013**, *130*, 4–50. doi:10.1016/j.jqsrt.2013.07.002.
- 1535 84. Hill, C.; Gordon, I.E.; Kochanov, R.V.; Barrett, L.; Wilzewski, J.S.; Rothman, L.S. HITRANonline: An
1536 online interface and the flexible representation of spectroscopic data in the HITRAN database. *Journal of*
1537 *Quantitative Spectroscopy and Radiative Transfer* **2016**, *177*, 4–14. doi:10.1016/j.jqsrt.2015.12.012.
- 1538 85. Skinner, F.M.; Gordon, I.E.; Hill, C.; Hargreaves, R.J.; Lockhart, K.E.; Rothman, L.S. Referencing Sources
1539 of Molecular Spectroscopic Data in the Era of Data Science: Application to the HITRAN and AMBDAS
1540 Databases. *Atoms* **2020**, *8*, 16. doi:10.3390/atoms8020016.
- 1541 86. Rothman, L.; Gordon, I.; Barber, R.; Dothe, H.; Gamache, R.; Goldman, A.; Perevalov, V.; Tashkun, S.;
1542 Tennyson, J. HITEMP, the high-temperature molecular spectroscopic database. *Journal of Quantitative*
1543 *Spectroscopy and Radiative Transfer* **2010**, *111*, 2139–2150. doi:10.1016/j.jqsrt.2010.05.001.
- 1544 87. Li, G.; Gordon, I.E.; Rothman, L.S.; Tan, Y.; Hu, S.M.; Kassi, S.; Campargue, A.; Medvedev, E.S.
1545 Rovibrational Line Lists for Nine Isotopologues of the CO Molecule in the X¹Σ⁺ Ground Electronic
1546 State. *The Astrophysical Journal Supplement Series* **2015**, *216*, 15. doi:10.1088/0067-0049/216/1/15.
- 1547 88. Hargreaves, R.J.; Gordon, I.E.; Rothman, L.S.; Tashkun, S.A.; Perevalov, V.I.; Lukashvskaya, A.A.;
1548 Yurchenko, S.N.; Tennyson, J.; Müller, H.S. Spectroscopic line parameters of NO, NO₂, and N₂O
1549 for the HITEMP database. *Journal of Quantitative Spectroscopy and Radiative Transfer* **2019**, *232*, 35–53.
1550 doi:10.1016/J.JQSRT.2019.04.040.
- 1551 89. Hargreaves, R.J.; Gordon, I.E.; Rey, M.; Nikitin, A.V.; Tyuterev, V.G.; Kochanov, R.V.; Rothman, L.S. An
1552 Accurate, Extensive, and Practical Line List of Methane for the HITEMP Database. *Astrophys. J. Suppl.*
1553 **2020**, *247*, 55. doi:10.3847/1538-4365/ab7a1a.
- 1554 90. Kochanov, R.; Gordon, I.; Rothman, L.; Shine, K.; Sharpe, S.; Johnson, T.; Wallington, T.; Harrison, J.;
1555 Bernath, P.; Birk, M.; Wagner, G.; Le Bris, K.; Bravo, I.; Hill, C. Infrared absorption cross-sections in
1556 HITRAN2016 and beyond: Expansion for climate, environment, and atmospheric applications. *Journal of*
1557 *Quantitative Spectroscopy and Radiative Transfer* **2019**, *230*, 172–221. doi:10.1016/J.JQSRT.2019.04.001.
- 1558 91. Karman, T.; Gordon, I.E.; van der Avoird, A.; Baranov, Y.I.; Boulet, C.; Drouin, B.J.; Groenenboom, G.C.;
1559 Gustafsson, M.; Hartmann, J.M.; Kurucz, R.L.; Rothman, L.S.; Sun, K.; Sung, K.; Thalman, R.; Tran, H.;
1560 Wishnow, E.H.; Wordsworth, R.; Vigasin, A.A.; Volkamer, R.; van der Zande, W.J. Update of the HITRAN
1561 collision-induced absorption section. *Icarus* **2019**, *328*, 160–175. doi:10.1016/J.ICARUS.2019.02.034.
- 1562 92. Kochanov, R.; Gordon, I.; Rothman, L.; Wcisło, P.; Hill, C.; Wilzewski, J. HITRAN Application Programming
1563 Interface (HAPI): A comprehensive approach to working with spectroscopic data. *Journal of Quantitative*
1564 *Spectroscopy and Radiative Transfer* **2016**, *177*, 15–30. Symposium on High Resolution Molecular Spectroscopy
1565 (HighRus-2015), Tomsk, Russia, doi:https://doi.org/10.1016/j.jqsrt.2016.03.005.
- 1566 93. Mikhailenko, S.; Barbe, A. High resolution infrared spectrum of ¹⁶O₃: The 3600–4300
1567 cm⁻¹ range reinvestigated. *J. Quant. Spectrosc. Radiat. Transfer* **2020**, *244*, 106823.
1568 doi:https://doi.org/10.1016/j.jqsrt.2019.106823.
- 1569 94. Starikova, E.; Barbe, A.; Tyuterev, V. The ν₃ bands of ¹⁷O¹⁷O¹⁸O and ¹⁷O¹⁸O¹⁷O ozone isotopomers. *J.*
1570 *Quant. Spectrosc. Radiat. Transfer* **2019**, *232*, 87–92. doi:10.1016/j.jqsrt.2019.05.002.
- 1571 95. Barbe, A.; Starikova, E.; De Backer, M.; Tyuterev, V. Analyses of infrared FT spectra of asymmetric ozone
1572 isotopologue ¹⁶O¹⁶O¹⁸O in the range 950–3850 cm⁻¹. *J. Quant. Spectrosc. Radiat. Transfer* **2018**, *218*, 231–247.
1573 doi:10.1016/j.jqsrt.2018.06.022.
- 1574 96. Tyuterev, V.; Kochanov, R.; Tashkun, S. Accurate ab initio dipole moment surfaces of ozone: First principle
1575 intensity predictions for rotationally resolved spectra in a large range of overtone and combination bands.
1576 *J. Chem. Phys.* **2017**, *146*, 064304. doi:10.1063/1.4973977.
- 1577 97. Tyuterev, V.; Barbe, A.; Jacquemart, D.; Janssen, C.; Mikhailenko, S.; Starikova, E. Ab initio predictions and
1578 laboratory validation for consistent ozone intensities in the MW, 10 and 5 μm ranges. *J. Chem. Phys.* **2019**,
1579 *150*. doi:10.1063/1.5089134.
- 1580 98. Boudon, V.; Champion, J.P.; Gabard, T.; Loëte, M.; Rotger, M.; Wenger, C. Spherical Top Theory and
1581 Molecular Spectra. In *Handbook of High-Resolution Spectroscopy*; Quack, M.; Merkt, F., Eds.; Wiley: Chichester,
1582 West Sussex, United Kingdom, 2011; Vol. 3, pp. 1437–1460.

- 1583 99. Wenger, C.; Boudon, V.; Rotger, M.; Sanzharov, J.P.; Champion, J.P. XTDS and SPVIEW: Graphical tools for
1584 the analysis and simulation of high-resolution molecular spectra. *Journal of Molecular Spectroscopy* **2008**,
1585 *251*, 102–113.
- 1586 100. Boudon, V.; Champion, J.P.; Gabard, T.; Loëte, M.; Michelot, F.; Pierre, G.; Rotger, M.; Wenger, C.; Rey,
1587 M. Symmetry-adapted tensorial formalism to model rovibrational and rovibronic spectra of molecules
1588 pertaining to various point groups. *J. Mol. Spectrosc.* **2004**, *228*, 620–634.
- 1589 101. Ba, Y.A.; Wenger, C.; Surleau, R.; Boudon, V.; Rotger, M.; Daumont, L.; Bonhommeau, D.A.; Tyuterev, V.G.;
1590 Dubernet, M.L. MeCaSDa and ECaSDa: Methane and ethene calculated spectroscopic databases for the
1591 virtual atomic and molecular data centre. *Journal of Quantitative Spectroscopy and Radiative Transfer* **2013**,
1592 *130*, 62–68.
- 1593 102. Person, W.; Krohn, B. Coriolis intensity perturbations of the ν_4 band of SF₆. *J. Mol. Spectrosc.* **1983**,
1594 *98*, 229–257.
- 1595 103. Aldridge, J.; Brock, E.; Filip, H.; Flicker, H.; Fox, K.; Galbraith, H.; Holland, R.; Kim, K.; Krohn, B.;
1596 Magnuson, D.; II, W.M.; owell, R.; Patterson, C.; Person, W.; Smith, D.; Werner, G. Measurement and
1597 analysis of the infrared-active stretching fundamental (ν_3) of UF₆. *J. Chem. Phys.* **1985**, *83*, 34–48.
- 1598 104. De Roure, D.; Jennings, N.R.; Shadbolt, N.R. The Semantic Grid: A Future e-Science Infrastructure. In *Grid*
1599 *Computing: Making the Global Infrastructure a Reality*; EPSRC/DTI Core e-Science Programme, 2001; pp. 437
1600 – 470. doi:10.1002/0470867167.
- 1601 105. Gruber, T. Toward principles for the design of ontologies used for knowledge sharing? *International Journal*
1602 *of Human-Computer Studies* **1995**, *43*, 907–928. doi:10.1006/ijhc.1995.1081.
- 1603 106. Lavrentiev, N.; Privezentsev, A.; Fazliev, A. Tabular and Graphic Resources in Quantitative Spectroscopy.
1604 In *Data Analytics and Management in Data Intensive Domains. DAMDID/RCDL 2018. Communications in*
1605 *Computer and Information Science*; Springer, 2019; Vol. 1003, pp. 55–69. doi:10.1007/978-3-030-23584-0_4.
- 1606 107. Lavrentiev, N.; Privezentsev, A.; Fazliev, A. Applied Ontologies for Managing Graphic Resources in
1607 Quantitative Spectroscopy. In *Data Analytics and Management in Data Intensive Domains DAMDID/RCDL*
1608 *2019. Communications in Computer and Information Science*; Springer, 2020; Vol. 1223, chapter 6.
1609 doi:10.1007/978-3-030-51913-1_6.
- 1610 108. Millar, T.J.; Bennett, A.; Rawlings, J.M.C.; Brown, P.D.; Charnley, S.B. Gas phase reactions and rate
1611 coefficients for use in astrochemistry - The UMIST ratfile. *Astron. Astrophys. Sup.* **1991**, *87*, 585–619.
- 1612 109. Dubernet, M.L.; Nenadovic, L. SPECTCOL: Spectroscopic and Collisional Data Retrieval. Astrophysics
1613 Source Code Library, record ascl:1111.005, 2011, p. 11005.
- 1614 110. Ba, Y.A.; Dubernet, M.L. The VAMDC SPECTCOL tool. *to be submitted to Atoms* **2020**.
- 1615 111. Srećković, V.A.; Ignjatović, L.M.; Jevremović, D.; Vujčić, V.; Dimitrijević, M.S. Radiative and Collisional
1616 Molecular Data and Virtual Laboratory Astrophysics. *Atoms* **2017**, *5*, 31.
- 1617 112. Ignjatovic, L.M.; Sreckovic, V.; Dimitrijevic, M. Photoionization of the alkali molecular ions in geo-cosmical
1618 plasmas. *Contrib. Astron. Obs. Skalnaté Pleso* **2020**, *50*, 187–192.
- 1619 113. Marinković, B.P.; Srećković, V.A.; Vujčić, V.; Ivanović, S.; Uskoković, N.; Nešić, M.; Ignjatović, L.M.;
1620 Jevremović, D.; Dimitrijević, M.S.; Mason, N.J. BEAMDB and MOLD—Databases at the Serbian Virtual
1621 Observatory for Collisional and Radiative Processes. *Atoms* **2019**, *7*, 11.
- 1622 114. Marinković, B.P.; Jevremović, D.; Srećković, V.A.; Vujčić, V.; Ignjatović, L.M.; Dimitrijević, M.S.; Mason, N.J.
1623 BEAMDB and MolD – databases for atomic and molecular collisional and radiative processes: Belgrade
1624 nodes of VAMDC. *The European Physical Journal D* **2017**, *71*. doi:10.1140/epjd/e2017-70814-6.
- 1625 115. Predojević, B.; Šević, D.; Marinković, B.P.; McEachran, R.P.; Blanco, F.; García, G.; Brunger, M.J. Joint
1626 theoretical and experimental study on elastic electron scattering from bismuth. *Phys. Rev. A* **2020**,
1627 *101*, 032704. doi:10.1103/PhysRevA.101.032704.
- 1628 116. McEachran, R.P.; Marinković, B.P.; García, G.; White, R.D.; Stokes, P.W.; Jones, D.B.; Brunger, M.J. Integral
1629 Cross Sections for Electron–Zinc Scattering over a Broad Energy Range (0.01–5000 eV). *Journal of Physical*
1630 *and Chemical Reference Data* **2020**, *49*, 013102. doi:10.1063/1.5135573.
- 1631 117. Marinković, B.; Bredehöft, J.; Vujčić, V.; Jevremović, D.; Mason, N. Rosetta Mission: Electron
1632 Scattering Cross Sections—Data Needs and Coverage in BEAMDB Database. *Atoms* **2017**, *5*, 46.
1633 doi:10.3390/atoms5040046.

- 1634 118. Marinković, B.P.; Pejčev, V.; Filipović, D.M.; Šević, D.; Milosavljević, A.R.; Milisavljević, S.; Rabasović, M.S.;
1635 Pavlović, D.; Maljković, J.B. Cross section data for electron collisions in plasma physics. *Journal of Physics:*
1636 *Conference Series* **2007**, *86*, 012006. doi:10.1088/1742-6596/86/1/012006.
- 1637 119. Denifl, S.; Garcia, G.; Huber, B.A.; Marinković, B.P.; Mason, N.; Postler, J.; Rabus, H.; Rixon, G.; Solovoyov,
1638 A.V.; Suraud, E.; Yakubovich, A.V. Radiation damage of biomolecules (RADAM) database development:
1639 current status. *Journal of Physics: Conference Series* **2013**, *438*, 012016. doi:10.1088/1742-6596/438/1/012016.
- 1640 120. Bartschat, K.; Zatsarinny, O. Benchmark calculations of atomic data for plasma and lighting applications.
1641 *Plasma Sources Science and Technology* **2011**, *20*, 024012. doi:10.1088/0963-0252/20/2/024012.
- 1642 121. Nina, A.; Radovanovic, M.; Srećković, V. *Integrations of satellite and ground-based observations and*
1643 *multi-disciplinarity in research and prediction of different types of hazards in Solar system, Book of abstracts;*
1644 Geographical Institute "Jovan Cvijić" of Serbian Academy of Sciences and Arts, 2019, Belgrade, 2019.
- 1645 122. Baratta, G.A.; Domingo, M.; G., F.; Leto, G.; Palumbo, M.E.; Satorre, M.A.; Strazzulla, G. Ion irradiation of
1646 CH₄-containing icy mixtures. *Nuclear Instruments and Methods in Physics Section B* **2003**, *209*, 283.
- 1647 123. Leto, G.; Baratta, G.A. Ly-alpha photon induced amorphization of Ic water ice at 16 Kelvin. Effects and
1648 quantitative comparison with ion irradiation. *A&A* **2003**, 397.
- 1649 124. Tennyson, J.; Yurchenko, S.N. ExoMol: molecular line lists for exoplanet and other atmospheres. *M. N. R.*
1650 *A. S.* **2012**, *425*, 21–33. doi:10.1111/j.1365-2966.2012.21440.x.
- 1651 125. Tennyson, J.; Hill, C.; Yurchenko, S.N. Data structures for ExoMol: Molecular line lists for exoplanet
1652 and other atmospheres. 6th international conference on atomic and molecular data and their
1653 applications ICAMDATA-2012. AIP, New York, 2013, Vol. 1545, *AIP Conference Proceedings*, pp. 186–195.
1654 doi:10.1063/1.4815853.
- 1655 126. Tennyson, J.; Yurchenko, S.N.; Al-Refaie, A.F.; Barton, E.J.; Chubb, K.L.; Coles, P.A.; Diamantopoulou, S.;
1656 Gorman, M.N.; Hill, C.; Lam, A.Z.; Lodi, L.; McKemmish, L.K.; Na, Y.; Owens, A.; Polyansky, O.L.; Rivlin,
1657 T.; Sousa-Silva, C.; Underwood, D.S.; Yachmenev, A.; Zak, E. The ExoMol database: molecular line lists for
1658 exoplanet and other hot atmospheres. *J. Mol. Spectrosc.* **2016**, *327*, 73–94. doi:10.1016/j.jms.2016.05.002.
- 1659 127. Tennyson, J.; Yurchenko, S.N.; Abd V. H. J. Clark and K. L. Chubb, A.F.A.R.; Conway, E.K.; Dewan, A.;
1660 Gorman, M.N.; Hill, C.; Lynas-Gray, A.E.; Mellor, T.; McKemmish, L.K.; Owens, A.; Polyansky, O.L.;
1661 Semenov, M.; Somogyi, W.; Tinetti, G.; Yu, A.U.; Waldmann, I.; Wang, Y.; Wright, S.; Yurchenko, O.P. The
1662 2020 release of the ExoMol database: molecular line lists for exoplanet and other hot atmospheres. *J. Quant.*
1663 *Spectrosc. Radiat. Transfer* **2020**, *255*, 107228. doi:10.1016/j.jqsrt.2020.107228.
- 1664 128. Lasis, A.A.; Oinas, V. *J. Geophys. Res.* **1991**, *96*, 9027.
- 1665 129. Bernath, P.F. MoLLIST: Molecular Line Lists, Intensities and Spectra. *J. Quant. Spectrosc. Radiat. Transfer*
1666 **2020**, *240*, 106687. doi:10.1016/j.jqsrt.2019.106687.
- 1667 130. Hill, C.; Dubernet, M.L.; Endres, C.; Karwasz, G.; Marinković, B.; Marquart, T.; Heinola, K.; Zwolf, C.M.;
1668 Moreau, N. Classification of Processes in Plasma Physics. Technical Report INDC(NDS)-0812, IAEA, 2020.
- 1669 131. Biémont, E.; Palmeri, P.; Quinet, P. A new database of astrophysical interest. *Astrophys. Space Sci.* **1999**,
1670 *635*, 269–270.
- 1671 132. Quinet, P.; Palmeri, P.; Biémont, E.; McCurdy, M.; Rieger, G.; Pinnington, E.; Wickliffe, M.; Lawler, J.
1672 Experimental and theoretical lifetimes, branching fractions and oscillator strengths in Lu II. *M. N. R. A. S.*
1673 **1999**, *307*, 934.
- 1674 133. Quinet, P.; Palmeri, P.; Biémont, E.; Li, Z.; Zhang, Z.; Svanberg, S. Radiative lifetime measurements and
1675 transition probability calculations in lanthanide ions. *J. Alloy. Compd.* **2002**, 344.
- 1676 134. Rahman, M.; Krishnakumar, E. Absolute partial and total electron ionization cross sections of uracil. *Int. J.*
1677 *Mass Spectrom* **2015**, *392*, 145–153. doi:10.1016/j.ijms.2015.10.003.
- 1678 135. Rahman, M.; Krishnakumar, E. Electron ionization of DNA bases. *J. Chem. Phys.* **2016**, *144*, 161102.
1679 doi:10.1063/1.4948412.
- 1680 136. Tadsare, V. Dissociative electron attachment to organic molecules. PhD thesis, Tata Institute of Fundamental
1681 Research, TIFR, Mumbai, India, 2018.
- 1682 137. Sinha, N.; Gupta, D.; Antony, B. Electron impact ionisation cross sections for complex molecules. *J. Phys.*
1683 *B: At. Mol. Opt. Phys.* **2019**, *52*, 145202. doi:10.1088/1361-6455/ab215a.
- 1684 138. Modak, P.; Antony, B. Electron scattering from FO. *J. Phys. B: At. Mol. Opt. Phys.* **2019**, *52*, 095202.
1685 doi:10.1088/1361-6455/ab13d2F.

- 1686 139. Nahar, S.; Antony, B. Review: Positron scattering from atoms and molecules. *Atoms* **2020**, *8*, 29.
1687 doi:10.3390/atoms8020029.
- 1688 140. Sinha, N.; Sahoo, A.; Antony, B. Positron scattering from pyridine and pyrimidine. *J. Phys. Chem. A* **2020**,
1689 *124*, 5147–5156. doi:10.1021/acs.jpca.0c02575.
- 1690 141. Modak, P.; Antony, B. Photoionization of CO using R-matrix theory. *Astrophys. J.* **2019**, *887*, 262.
1691 doi:10.3847/1538-4357/ab5583.
- 1692 142. Modak, P.; Antony, B. Probing photon interaction with H₂O and D₂O. *J. Phys. B: At. Mol. Opt. Phys.* **2020**,
1693 *53*, 045202. doi:10.1088/1361-6455/ab5904.
- 1694 143. Kwon, D.H.; Savin, D.W. Electron-impact ionization of P-like ions forming Si-like ions. *ApJ* **2014**, *784:13*, 1–7.
1695 doi:10.1088/0004-637X/784/1/13.
- 1696 144. Kwon, D.H.; Savin, D.W. Effects of configuration interaction for dielectronic recombination of Na-like ions
1697 forming Mg-like ions. *ApJ* **2011**, *734:2*, 1–7. doi:10.1088/0004-637X/734/1/2.
- 1698 145. Kim, D.S.; Kwon, D.H. Theoretical photoionization spectra for Mg-isoelectronic Cl⁵⁺ and Ar⁶⁺ ions. *J.*
1699 *Phys. B: At. Mol. Opt. Phys.* **2015**, *48:105004*, 1–11. doi:10.1088/0953-4075/48/10/105004.
- 1700 146. Zhang, D.H.; Kwon, D.H. Theoretical electron-impact ionization of W¹⁷⁺ forming W¹⁸⁺. *J. Phys. B: At.*
1701 *Mol. Opt. Phys.* **2014**, *47:075202*, 1–6. doi:10.1088/0953-4075/47/7/075202.
- 1702 147. Kwon, D.H. Dielectronic recombination of lowly charged tungsten ions W^{q+} ($q = 5 - 10$). *J. Quant.*
1703 *Spectrosc. Radiat. Transfer* **2018**, *208*, 64–70. doi:10.1016/j.jqsrt.2018.01.005.
- 1704 148. Chai, K.B.; Kwon, D.H. Optical emission spectroscopy and collisional-radiative modeling for
1705 low temperature Ar plasmas. *J. Quant. Spectrosc. Radiat. Transfer* **2019**, *227*, 136–144.
1706 doi:10.1016/j.jqsrt.2019.02.015.
- 1707 149. Ralser, S.; Postler, J.; Harnisch, M.; Ellis, A.M.; Scheier, P. Extracting cluster distributions from mass spectra:
1708 IsotopeFit. *International journal of mass spectrometry* **2015**, *379*, 194–199. doi:10.1016/j.ijms.2015.01.004.
- 1709 150. Scheier, P.; Märk, T. Doubly charged argon clusters and their critical size. *The Journal of chemical physics*
1710 **1987**, *86*, 3056–3057. doi:10.1063/1.452013.
- 1711 151. Schöbel, H.; Bartl, P.; Leidlmair, C.; Denifl, S.; Echt, O.; Märk, T.; Scheier, P. High-resolution mass
1712 spectrometric study of pure helium droplets, and droplets doped with krypton. *The European Physical*
1713 *Journal D* **2011**, *63*, 209–214. doi:10.1140/epjd/e2011-10619-1.
- 1714 152. Regandell, S.; Marquart, T.; Piskunov, N. Inside a VAMDC data node - putting standards into practical
1715 software. *Physica Scripta* **2018**, *93*, 035001, [arXiv:astro-ph.IM/1803.09217]. doi:10.1088/1402-4896/aaa268.
- 1716 153. Zwölf, C.M.; Moreau, N.; Dubernet, M.L. New model for datasets citation and extraction
1717 reproducibility in VAMDC. *Journal of Molecular Spectroscopy* **2016**, *327*, 122–137, [arXiv:cs.DL/1606.00405].
1718 doi:10.1016/j.jms.2016.04.009.
- 1719 154. Walton, N.; Astrogrid Consortium. Meeting the User Science Challenge for a Virtual Universe. Toward an
1720 International Virtual Observatory; Quinn, P.J.; Górski, K.M., Eds., 2004, p. 187. doi:10.1007/10857598_29.
- 1721 155. Moreau, N.; Zwölf, C.M.; Ba, Y.A.; Richard, C.; Boudon, V.; Dubernet, M.L. The VAMDC Portal as a Major
1722 Enabler of Atomic and Molecular Data Citation. *Galaxies* **2018**, *6*, 105. doi:10.3390/galaxies6040105.
- 1723 156. Taylor, M.B.; Boch, T.; Taylor, J. SAMP, the Simple Application Messaging Protocol: Letting
1724 applications talk to each other. *Astronomy and Computing* **2015**, *11*, 81–90, [arXiv:astro-ph.IM/1501.01139].
1725 doi:10.1016/j.ascom.2014.12.007.
- 1726 157. Heller, S.; McNaught, A.; Pletnev, I.; Stein, S.; Tchekhovskoi, D. InChI, the IUPAC International Chemical
1727 Identifier. *J. Cheminform.* **2015**, pp. 7–23. doi:10.1186/s13321-015-0068-4.
- 1728 158. Zwölf, C.; Moreau, N.; Yaya-Awa, B.; Dubernet, M.L. Implementing in the VAMDC the New Paradigms for
1729 Data Citation from the Research Data Alliance. *Data Science Journal* **2018**, *1*, 4. doi:10.5334/dsj-2019-004.
- 1730 159. Rey, M.; Nikitin, A.V.; Babikov, Y.L.; Tyuterev, V.G. TheoReTS – An information system for theoretical
1731 spectra based on variational predictions from molecular potential energy and dipole moment surfaces. *J.*
1732 *Mol. Spectrosc.* **2016**, *327*, 138–158. doi:10.1016/j.jms.2016.04.006.
- 1733 160. Huang, X.; Schwenke, D.W.; Lee, T.J. Quantitative validation of Ames IR intensity and new line lists
1734 for ^{32/33/34}S¹⁶O₂, ³²S¹⁸O₂ and ¹⁶O³²S¹⁸O. *J. Quant. Spectrosc. Radiat. Transfer* **2019**, *225*, 327 – 336.
1735 doi:10.1016/j.jqsrt.2018.11.039.
- 1736 161. Owens, A.; Yachmenev, A.; Tennyson, J.; Thiel, W.; Yurchenko, S.N. ExoMol Molecular line lists XXIX:
1737 The rotation-vibration spectrum of methyl chloride up to 1200 K. *M. N. R. A. S.* **2018**, *479*, 3002–3010.
1738 doi:10.1093/mnras/sty1542.

- 1739 162. Rey, M.; Chizhmakova, I.; Nikitin, A.; Tyuterev, V. Understanding global infrared opacity and hot bands of
1740 greenhouse molecules with low vibrational modes from first-principles calculations: The case of CF₄. *Phys.*
1741 *Chem. Chem. Phys.* **2018**, *20*, 21008–21033. doi:10.1039/c8cp03252a.
- 1742 163. Egorov, O.; Nikitin, A.; Rey, M.; Rodina, A.; Tashkun, S.; Tyuterev, V. Global modeling of NF₃ line
1743 positions and intensities from far to mid-infrared up to 2200 cm⁻¹. *J. Quant. Spectrosc. Radiat. Transfer* **2019**,
1744 *239*, 106668. doi:10.1016/j.jqsrt.2019.106668.
- 1745 164. Rey, M.; Nikitin, A.V.; Tyuterev, V.G. Accurate Theoretical Methane Line Lists in the Infrared up to 3000 K
1746 and Quasi-continuum Absorption/Emission Modeling for Astrophysical Applications. *ApJ* **2017**, *847*, 105.
- 1747 165. Yurchenko, S.N.; Amundsen, D.S.; Tennyson, J.; Waldmann, I.P. A hybrid line list for CH₄ and hot methane
1748 continuum. *A&A* **2017**, *605*, A95. doi:10.1051/0004-6361/201731026.
- 1749 166. Wong, A.; Bernath, P.; Rey, M.; Nikitin, A.; Tyuterev, V. Atlas of Experimental and Theoretical
1750 High-temperature Methane Cross Sections from T = 295 to 1000 K in the Near-infrared. *Astrophys.*
1751 *J. Suppl.* **2019**, *240*. doi:10.3847/1538-4365/aaed39.
- 1752 167. Erard, S.; Cecconi, B.; Le Sidaner, P.; Berthier, J.; Henry, F.; Molinaro, M.; Giardino, M.; Bourrel, N.; André,
1753 N.; Gangloff, M.; et al.. The EPN-TAP protocol for the Planetary Science Virtual Observatory. *Astronomy*
1754 *and Computing* **2014**, *7-8*, 52–61. doi:10.1016/j.ascom.2014.07.008.
- 1755 168. van der Tak, F.F.S.; Lique, F.; Faure, A.; Black, J.H.; van Dishoeck, E.F. The Leiden Atomic and
1756 Molecular Database (LAMDA): Current Status, Recent Updates, and Future Plans. *Atoms* **2020**, *8*, 15.
1757 doi:10.3390/atoms8020015.
- 1758 169. Endres, C.P.; Martin-Drumel, M.A.; Zingsheim, O.; Bonah, L.; Pirali, O.; Zhang, T.; Sánchez-Monge, Á.;
1759 Möller, T.; Wehres, N.; Schilke, P.; McCarthy, M.C.; Schlemmer, S.; Caselli, P.; Thorwirth, S. SOLEIL and
1760 ALMA views on prototypical organic nitriles: C₂H₅CN. *J. Mol. Spectrosc.* **2020**, *submitted*.
- 1761 170. Möller, T.; Endres, C.; Schilke, P. eXtended CASA Line Analysis Software Suite (XCLASS). *A&A* **2017**,
1762 *598*, A7. doi:10.1051/0004-6361/201527203.
- 1763 171. Möller, T.; Bernst, I.; Panoglou, D.; Muders, D.; Ossenkopf, V.; Röllig, M.; Schilke, P. Modeling
1764 and Analysis Generic Interface for eXternal numerical codes (MAGIX). *A&A* **2013**, *549*, A21.
1765 doi:10.1051/0004-6361/201220063.
- 1766 172. Moscadelli, L.; Rivilla, V.M.; Cesaroni, R.; Beltrán, M.T.; Sánchez-Monge, Á.; Schilke, P.; Mottram, J.C.;
1767 Ahmadi, A.; Allen, V.; Beuther, H.; Csengeri, T.; Etoke, S.; Galli, D.; Goddi, C.; Johnston, K.G.; Klaassen,
1768 P.D.; Kuiper, R.; Kumar, M.S.N.; Maud, L.T.; Möller, T.; Peters, T.; Van der Tak, F.; Vig, S. The feedback of an
1769 HC HII region on its parental molecular core. The case of core A1 in the star-forming region G24.78+0.08.
1770 *A&A* **2018**, *616*, A66. doi:10.1051/0004-6361/201832680.
- 1771 173. Dimitrijević, M.S.; Sahal-Bréchet, S. On the Application of Stark Broadening Data Determined with a
1772 Semiclassical Perturbation Approach. *Atoms* **2014**, *2*, 357–377.
- 1773 174. Dreizler, S. HST Spectroscopy of PG 1159 Stars: the Boundary of the GW VIR Instability Strip. *Baltic*
1774 *Astronomy* **1998**, *7*, 71–82.
- 1775 175. Dojčinović, I.P.; Trklja, N.; Tapalaga, I.; Purić, J. Investigation of Stark line broadening within
1776 spectral series of potassium and copper isoelectronic sequences. *M. N. R. A. S.* **2019**, *489*, 2997–3002.
1777 doi:10.1093/mnras/stz2367.
- 1778 176. Lavrentyev, N.; Makogon, M.; Fazliev, A. Comparison of the HITRAN and GEISA Spectral Databases
1779 Taking into Account the Restriction on Publication of Spectral Data. *Atmospheric and Oceanic Optics* **2011**,
1780 *24*, 436–451. doi:10.1134/S1024856011050113.
- 1781 177. Wilkinson, M.D.; Dumontier, M.; Aalbersberg, I.J.; Appleton, G.; Axton, M.; Baak, A.; Blomberg, N.;
1782 Boiten, J.W.; da Silva Santos, L.B.; Bourne, P.E.; Bouwman, J.; Brookes, A.J.; Clark, T.; Crosas, M.; Dillo, I.;
1783 Dumon, O.; Edmunds, S.; Evelo, C.T.; Finkers, R.; Gonzalez-Beltran, A.; Gray, A.J.G.; Groth, P.; Goble, C.;
1784 Grethe, J.S.; Heringa, J.; 't Hoen, P.A.C.; Hooft, R.; Kuhn, T.; Kok, R.; Kok, J.; Lusher, S.J.; Martone, M.E.;
1785 Mons, A.; Packer, A.L.; Persson, B.; Rocca-Serra, P.; Roos, M.; van Schaik, R.; Sansone, S.A.; Schultes, E.;
1786 Sengstag, T.; Slater, T.; Strawn, G.; Swertz, M.A.; Thompson, M.; van der Lei, J.; van Mulligen, E.; Velterop,
1787 J.; Waagmeester, A.; Wittenburg, P.; Wolstencroft, K.; Zhao, J.; Mons, B. The FAIR Guiding Principles for
1788 scientific data management and stewardship. *Scientific Data* **2016**, *3*, 160018. doi:10.1038/sdata.2016.18.
- 1789 178. Lavrentiev, N.; Rodimova, O.; Fazliev, A. Systematization of published scientific graphics characterizing
1790 the water vapor continuum absorption: I. Publications of 1898-1980. 24-th International Symposium on
1791 Atmospheric and Oceanic Optics: Atmospheric Physics, 2018. doi:10.1117/12.2504325.

- 1792 179. Lavrentiev, N.; Rodimova, O.; Fazliev, A. Systematization of graphically plotted published spectral
1793 functions of weakly bound water complexes. 22-nd International Symposium on Atmospheric and Oceanic
1794 Optics: Atmospheric Physics, 2016. doi:10.1117/12.2249159.
- 1795 180. Laverick, M.; Lobel, A.; Merle, T.; Royer, P.; Martayan, C.; David, M.; Hensberge, H.; Thienpont, E. The
1796 Belgian repository of fundamental atomic data and stellar spectra (BRASS). I. Cross-matching atomic
1797 databases of astrophysical interest. *A&A* **2018**, *612*, A60. doi:10.1051/0004-6361/201731933.
- 1798 181. See <http://dataosu.obs-besancon.fr>.
- 1799 182. Atherton, C.J.; Barton, T.; Basney, J.; Broeder, D.; Costa, A.; van Daalen, M.; Dyke, S.; Elbers, W.; Enell,
1800 C.F.; Fasanelli, E.M.V.; Fernandes, J.; Florio, L.; Gietz, P.; Groep, D.L.; Junker, M.B.; Kanellopoulos, C.;
1801 Kelsey, D.; Kershaw, P.; Knapic, C.; Kollegger, T.; Koranda, S.; Linden, M.; Marinic, F.; Matyska, L.;
1802 Nyrönen, T.H.; Paetow, S.; Paglione, L.A.D.; Parlati, S.; Phillips, C.; Prochazka, M.; Rees, N.; Short, H.;
1803 Stevanovic, U.; Tartakovsky, M.; Venekamp, G.; Vitez, T.; Wartel, R.; Whalen, C.; White, J.; Zwölf, C.M.
1804 Federated Identity Management for Research Collaborations. Standard, Research Data Alliance, 2019.
1805 doi:10.5281/zenodo.1307551.
- 1806 183. Zwölf, C.M.; Rixon, G. Authentication, Authorisation and Accounting strategy. Technical deliverable,
1807 VAMDC Consortium, 2015. doi:10.5281/zenodo.3936606.
- 1808 184. Wittenburg, P.; Hellström, M.; Zwölf, C.M.; Abroshan, H.; Asmi, A.; Di Bernardo, G.; Couvreur, D.; Gaizer,
1809 T.; Holub, P.; Hoof, R.; Häggström, I.; Kohler, M.; Koureas, D.; Kuchinke, W.; Milanese, L.; Padfield,
1810 J.; Rosato, A.; Staiger, C.; van Uytvanck, D.; Weigel, T. Persistent identifiers: Consolidated assertions.
1811 Standard, Research Data Alliance, 2017. doi:10.5281/zenodo.1116189.
- 1812 185. Collins, S.; Genova, F.; Harrower, N.; Hodson, S.; Jones, S.; Laaksonen, L.; Mietchen, D.; Petruskaitė, R.;
1813 Wittenburg, P. Turning FAIR into reality - Final report and action plan from the European Commission
1814 expert group on FAIR data. Report, Publications Office of the European Union, 2018. doi:10.2777/1524.
- 1815 186. Berners-Lee, T.; Hendler, J.; Lassila, O. Toward principles for the design of ontologies used for knowledge
1816 sharing. *The Semantic Web* **2001**, *43*, 907–928.
- 1817 187. Group, W.O.W. *OWL 2 Web Ontology Language Document Overview, W3C Recommendation 27*
1818 *October 2009*. The World Wide Web Consortium (W3C), <https://www.w3.org/>, 1 ed., 2009.
1819 <http://www.w3.org/TR/2009/REC-owl2-overview-20091027/>.
- 1820 188. Privezentsev, A.; Tsarkov, D.; Fazliev, A.; Tennyson, J. Computed Knowledge Base for Description of
1821 Information Resources of Water Spectroscopy. 7th International Workshop on OWL: Experiences and
1822 Directions (OWLED 2010), 2010.
- 1823 189. Fazliev, A.; Privezentsev, A.; Tsarkov, D.; Tennyson, J. Ontology-Based Content Trust Support
1824 of Expert Information Resources in Quantitative Spectroscopy. In *Knowledge Engineering and the*
1825 *Semantic Web, Communications in Computer and Information Science*; Springer, 2013; Vol. 394, pp. 15–28.
1826 doi:10.1007/978-3-642-41360-5_2.
- 1827 190. Voronina, V.; Privezentsev, A.; Tsarkov, D.; Fazliev, A. An Ontological Description of States and Transitions
1828 in Quantitative Spectroscopy. XX-th International Symposium on Atmospheric and Ocean Optics:
1829 Atmospheric Physics, 2014. doi:10.1117/12.2075512.
- 1830 191. Akhlestin, A.; Lavrentiev, N.; Rodimova, O.; Fazliev, A. The continuum absorption: trust assessment
1831 of published graphical information. 25-th International Symposium on Atmospheric and Ocean Optics:
1832 Atmospheric Physics, 2019. doi:10.1117/12.2541741.