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International Atomic and Molecular Code Centres Network: Virtual Atomic and Molecular Data Centres Consortium Annual Meeting

Summary Report of the 8th Biennial Technical Meeting of the Code Centres Network

IAEA Headquarters, Vienna, Austria
15 – 17 November 2023

Prepared by

C. Hill
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Vienna, Austria

November 2023

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ABSTRACT

The International Code Centres Network (CCN) is a group of experts developing codes and models for atomic, molecular and plasma-surface interaction data relevant to fusion applications. Variable subsets of the group are brought together by the IAEA Atomic and Molecular Data (AMD) Unit in order to discuss computational and scientific issues associated with code developments. At the 8th Technical Meeting described in this report, which was held virtually from 15 – 17 November 2023, 31 experts in the field of atomic and molecular physics met, representing 23 databases within the Virtual Atomic and Molecular Data Centres (VAMDC) Consortium. The VAMDC brings together research institutions that share a common technical and political framework for the distribution and curation of atomic and molecular data; this virtual meeting was its annual meeting at which priorities for data and software infrastructure development are planned and membership within the collaboration for the coming year established.

November 2023

Table of Contents

1. Introduction

The International Code Centres Network (CCN) is coordinated by the IAEA Atomic and Molecular Data (AMD) Unit in order to gather, compare, validate, and provide access to computational codes relevant for modellers in fusion and plasma sciences. Since 2005, the Unit has organized a series of meetings of code developers in the CCN to address code-related issues including the accessibility of physics codes.

The Virtual Atomic and Molecular Data Centres Consortium is a consortium of Institutes and Research Institutions that share a common technical and political framework for the distribution and curation of atomic and molecular data.

The VAMDC Consortium's technical framework relies on the use of the e-science VAMDC infrastructure that provides the international research community with access to a broad range of atomic and molecular (A&M) data compiled within a set of A&M databases accessible through the provision of a single portal. Furthermore VAMDC aims to provide A&M data providers and compilers with a large dissemination platform for their work.

The VAMDC Consortium's political framework relies on rules of collaboration and organisation that are described in a Memorandum of Understanding (MoU) and in its Internal Regulations documents, available at https://vamdc.org/structure/organisation/.

The VAMDC Consortium Activities are defined as (see Article 2.1 of the MoU):

- distribution, curation, access to atomic and molecular data through the "VAMDC Infrastructure" as defined in the Internal Regulations document;
- maintenance, upgrade and evolution of the "VAMDC Infrastructure";
- promotion of scientific evaluation/validation of atomic and molecular data;
- promotion of scientific activities linked to the production of atomic and molecular data;
- promotion of access to data with different users: research, education, business, outreach;
- organisation of meetings open to external people;
- specification of VAMDC-XSAMS standards and extensions thereto.

Since 2014 the VAMDC Consortium has been managed by a board of directors composed of the full members of the Consortium (definitions given in the MoU) and by a Science and Technical Board composed of the scientific and technical representatives of each database included in the infrastructure and of experts (full members and associated members of the VAMDC Consortium). The Board of Directors manages the political structure of the VAMDC Consortium; the Science and Technical Board manages the VAMDC e-infrastructure and ensures the maintenance and the various technological developments.

This report documents the 8th CCN meeting, which was held virtually, and functioned as the annual meeting of the VAMDC Consortium for 2023. The following section contains the meeting summary, database node summaries, and plans for the coming year. Appendices 1 and 2 list the participants and the meeting agenda. The current memberships of the Board of Directors and the Scientific and Technical Board are given in Appendices 3 and 4; a list of the current VAMDC databases forms Appendix 5.

2. Meeting Summary

2.1 VAMDC database node reports: status and updates

The VAMDC Consortium comprises a set a database nodes, connected through the portal at https://portal.vamdc.org/vamdc_portal/home.seam. The status of each node reported at this meeting is reported below. Further details of all the VAMDC nodes is given in Appendix 5.

*CaSDa

- *CaSDa is a suite of nine databases for the calculated spectra of nine polyatomic molecules, mostly of tetrahedral or octahedral symmetry.
- The latest calculations, for silane (SiH_4), will be released soon.
- There is an ongoing problem with the retrieving of large datasets, since these line lists can be large; proposed solutions are to provide SQLite output or to adopt the ExoMol output format.

BASECOL

- A new partner group, led by Otoniel Denis Alpizar at Universidad Autónoma de Chile will deploy a mirror of this database.
- Ultimately, responsibility for BASECOL may transfer to Chile.
- The BASECOL node output has been revised to better match the BASECOL website service.

BEAMDB, MolD and ASCol

- Active and running as VAMDC nodes.
- The BEAMDB database has 3-D plotting capability, raising the question of whether this can be deployed more widely throughout the VAMDC.
- Funding is assured for the next three years.

CDMS

- New data has been included.
- There is currently some funding support for the project: half-FTE scientists
- There is ongoing concern about the status of the physical server and the database and its infrastructure may move to the cloud.
- There is a longer-term (2–3 year plan to include experimental data in CDMS, but this would require an expansion to its data model; CDMS is expected to stay within the VAMDC Consortium.
- Planned action will start soon to solve reported issues with the CDMS node output

CHIANTI

- Nothing to report, service still running.

HITRAN

- The VAMDC version of this database is HITRAN-2020; HITRAN-2024 is due soon.
- The software stack for the web service was recently updated, but broke compatibility with the VAMDC node software; the latest fixes to this, implemented by the University of Cambridge group, should fix this by supporting compatibility with the latest version of he Django package.

IDEADB

- The IDEADB node has been inactive for some time, but came back online recently.
- Bratislav Marinkovic contacted Johannes Postler, who tried to contact the University of Innsbruck in relation to the database but got no reply.
- It would be possible to incorporate IDEADB into one of the Belgrade databases run by Bratislav Marinkovic and no objection from Innsbruck is anticipated.

KFE

- The Data Center for Plasma Physics at the Korea Institute of Fusion Energy (KFE) maintains a Web Database System for collision cross-sections, rate coefficients, electron collisions and heavy particle reactions as well as numerical and bibliographic data, with a focus on fusion energy research.
- The database can already output data in XSAMS format, but without states description.
- Initially a VAMDC associated member, KFE will seek ways to connect data in order to become a full member. Hosting by commercial cloud services could be a solution to existing security concerns; a snapshot node and container, as for the PEARL database could also be a solution.
- KFE also has more than 100,000 DFT calculations of molecular structures and collision cross sections; deploying these as a VAMDC node would be challenge both from an administrative and software development perspective.

KIDA

- Technical maintenance is now complete, leaving more time to spend on the data content of the database.
- KIDA is consulting with its user community to establish how the database will evolve in future; this may affect VAMDC compatibility.
- There is the possibility of deploying apps to display KIDA data in comparison with UdfA data, should that database be reconnected to the VAMDC.

NIFS

- The NIFS database is continuously updated but the VAMDC version deployed as a node is not updated and is missing about 2/3 of the available records.
- The VAMDC version also misses the bibliography and state descriptions.
- 1 FTE scientist is in-post for adding new data, but there is little ongoing effort for VAMDC developments.

- "Classical" VALD has hyperfine structure for the majority of lines in the database; this is not yet in the "VAMDC-VALD" deployment serving as a VAMDC node. This is because

NIST-ASD

- Version 5.11 of the database will be released at the end of November 2023, to include He-like ions and more than 300,000 lines.
- Currently the VAMDC node maintainers are not receiving alerts when connectivity problems occur: Paris Observatory will look into this.

PEARL

- PEARL (Photonic Electronic Atomic Reaction Library) is a database of photoionization/electron-impact ionization and dielectronic recombination cross sections and rate coefficients maintaned by the Atomic Data Center of the Korea Atomic Energy Research Institute (KAERI).
- There is no VAMDC web service yet (i.e. PEARL does not function as a VAMDC node).
- It was agreed that PEARL could, if agreed with KAERI, move forward with deployment of a node elsewhere (Cambridge?) based on exported snapshots and containers; there is a need to agree an update schedule so that the "snapshot node" stays current.

Stark-B

- Stark-B is still receiving updates, but may freeze when the present data maintainers cease work on it.

TipTopBase

- No change, but a replacement, larger database is proposed, which will be deployed as a new VAMDC node.

VALD-Moscow

- "Classical" VALD has hyperfine structure for the majority of lines in the database; this is not yet in the "VAMDC-VALD" deployment serving as a VAMDC node. This is because the "Classical" service calculates it on request: can this be done with the VAMDC node?

VALD-Uppsala

- Data entry continues on "Classical" VALD.
- The loss of a maintainer and obsolete infrastructure has compromised the node software: it is hoped that the database can be reworked using SQLite.
- The VAMDC node is running, but is "years out of date" with respect to "Classical" VALD; difficult software issues (importing data) make it difficult to bring up to date, something that would be solved in the move to SQLite.

2.2 Procedures for adopting a new node within the VAMDC

Nicolas Moreau outlined the procedures for connecting a new database node service to the VAMDC infrastructure:

- Start with request to support@vamdc.org
- There is a technical checking procedure, which needs to be more rigorous.
- Better science evaluation is also required.
- Node registration needs a password, currently held by Nicolas Moreau (Paris Observatory), Carlo Zwölf (Paris Observatory) and Guy Rixon (University of Cambridge).

The question of metadata-only nodes was raised:

- This needs to be discussed and approved by the BoD.
- it would also require a new kind of portal for the metadata search.
- See https://vespa.obspm.fr/planetary/data/

2.3 Procedures for removing VAMDC partners

Generally, VAMDC partners are not removed from the Consortium by the BoD, but may choose to resign; in practice they generally just go silent. The Board could contact inactive members regularly to verify they intend to continue within the VAMDC. In principle, the BoD could eject a defaulting member, but no good definition of "defaulting" exists at present.

It was proposed that full VAMDC members should be required to maintain a science contact in addition to a technical contact, it order to answer user questions about their database nodes. There is a continued need for node operators to be proactive about reporting their problems: *if their node doesn't work, it should be marked inactive until it is fixed*.

2.4 Reporting issues and technical support within the VAMDC

Marie-Lise Dubernet (Paris Observatory) noted that several issues have recently been found with either the interpretation of VSS2 queries by some nodes or in their XSAMS output. It was agreed that there should be a mechanism for reporting issues and keeping users informed of when these issues are under consideration; GitHub provides this functionality and is one solution, though apparently some users do not have experience with it.

There is also a need to reform the process of adding species to the VAMDC Species Database: errors (for example, in charge or mass) upon entry of a species into the database cannot be over-ridden by other databases but instead require central management. Furthermore, some databases include the charge in the stoichiometric formula whereas others do not. It was noted that the PyValem library can help standardise this process by automatically assigning charge and mass given a valid species specification string, and this will be investigated by Nicolas Moreau at Paris Observatory.

Feed-through of query data from the VAMDC Query Store to Zenodo is implemented but currently unused because of minor issues, including incorrectly-formatted references; this should be fixed soon because it is an important functionality for HITRAN and BASECOL, in particular.

2.5 Extensions to the XSAMS Schema

2.5.1 Extensions required for the PAH database

Giacomo Mulas (Osservatorio Astronomico di Cagliari) proposed extensions to the XSAMS Schema to cater for the specific needs of the PAH database:

- The tabulated data type to be extended to cover theoretical spectra.
- There is a need for a tabulated polarizability tensor: good for aligned molecules and for correlated absorption and scattering data (real and imaginary parts of the same tensor); this requires either a complex data types or link between two structures with real data. An averaged polarizability data type would also be helpful.
- Add an optional precursor field to cross section types.

A Working Group, lead by Giacomo Mulas, was proposed to implement these changes:
- Guy Rixon (to assist with coding the new feature into the XSAMS generator)
- Christian Hill (to assist with the XSAMS Schema)
- Thomas Marquart (to assist with node software in a time-limited capacity)

2.5.2 Extensions and corrections to the case-by-case molecular state schema

Marie-Lise Dubernet (Paris Observatory) raised several issues related to the "case-by-case" Schema for molecular states:

- A request for a `SpinComponentLabel` and `Omega` entries for the `lpos` ("linear polyatomic, open-shell") case, to allow for both Hund's case (a)- and case (b)-type angular momentum coupling schemes.

- A request for a `rotorSym` element for labelling the symmetry of the rotational-torsional component of the wavefunction for `stcs` ("symmetric top, closed-shell") case molecules. There should, at a minimum, be generic symmetry labels and generic quantum numbers (named by attribute) for every molecular state "case".

2.6 The VAMDC website

Yaye-Awa Ba (Paris Observatory) reported on the current status of the VAMDC website:

- The website currently runs on WordPress 6.2 and PHP, with a large number of plugins essential to make it work.
- Security updates are applied frequently (2 – 3 times per year), sometimes leading to compatibility issues with plugins.

- Content update is easy if it doesn't change the site structure (only leaf nodes added and no changes in sub-tabs), otherwise it is potentially very hard.
- Off-site replicas of the website exist; DNS changes would be required to use them.
- There is a need to clean out outdated content and update relevant pages (for example, documentation pages for the node software).

2.7 Machine Learning experiences with VAMDC output

Thomas Marquart (Uppsala University) reported on experiments he has carried out using ChatGPT 4. This service, from OpenAI (https://openai.com/) is good at introspecting XSAMS output and can plot meaningful charts from the data such documents contain as well as generating Python code to reproduce its plots. It was found to be less successful at generating VSS2 queries, and cannot directly query the VAMDC portal. Verification of the results is a problem, but one can verify the Python code more robustly than individual transformation of specific XSAMS files.

It is possible to add custom APIs to a special instance of ChatGPT that is pre-trained and shared with users, but is a paid-for service from OpenAI. It was noted that both France and Germany will have similar academic AI services soon and these could be utilised for this purpose more cost-effectively.

If the manual transcription of the PEARL database runs into problems, work on this could be paused and attempted with AI to save effort.

2.8 LXCat

Daan Boer (Eindhoven University of Technology) reported on developments to the LXCat database of low-temperature electron–ion collisional data. This database is not currently part of the VAMDC but has recently undergone an extensive overhaul to its software infrastructure. LXCat is now based on a hierarchical JSON data schema using the ArangoDB graph database system, the Zod schema declaration and validation library, and the Citation.js library to manage references. Work on describing different atomic and molecular states is ongoing but the major LJ and j-j coupling schemes are implemented.

It was noted that transcription from LXCat to XSAMS format should be possible where states are fully-specified and that it might even be possible to add the LXCat format as an alternative output format for VAMDC nodes, though this would require substantial software development work.

2.9 CollisionDB and PyValem

Christian Hill gave a demonstration of the new CollisionDB database of plasma collisional processes developed at the IAEA (to be deployed at https://amdis.iaea.org/db/collisiondb/). At the time of writing, this database contains 122,458 cross sections and rate coefficients. An explanation of the JSON metadata format and timestamping / provenance policies was given. Atomic and molecular species and states are described using the notation implemented by the PyValem Python library (https://github.com/xnx/pyvalem), which could be adopted more

widely by the VAMDC to remove ambiguity around the specification of atoms, molecules and their quantum states (see above).

2.10 Outreach and future plans for VAMDC

Some discussion took place concerning potential future activities of the VAMDC, with a focus on two particular areas: machine learning and the provision of educational resources based on VAMDC data.

2.10.1 Datasets for Machine Learning applications

The databases connected through the VAMDC infrastructure output their data in a consistent format, compliant with the well-described XSAMS Schema and could be exploited effectively by machine learning (ML) algorithms to facilitate data transformation, visualization and, potentially, the generation of data otherwise missing from the data sets.

XML is not ideally suited to ML applications, however, being verbose and having content spread across syntactically different parts of the markup (for example, elements and attributes). It would be possible to transform the XML into a flatter format (perhaps with the help of a large language model service such as ChatGPT) and to make available a large amount of VAMDC data for exploitation by ML projects. There would be a cost (storage, bandwidth) but the developer time required need not be all that great.

2.10.2 Educational resources from VAMDC databases

Although limited available resources do not currently allow VAMDC Consortium members to develop comprehensive educational content in a consistent format for distribution on the VAMDC website, an easier start could be made by making the metadata for each database available in this way: for example, a list of the species and processes for which data is obtainable from each node.

A limited number of educational resources, for example in the form of Jupyter Notebooks, could also be made available in this way; already some databases (including HITRAN and VALD) are widely used in both graduate and undergraduate courses and providing such resources may be an effective way of promoting usage of the VAMDC services in general.

Appendix 1: Meeting Participants

Yaye Awa BA, Observatoire de Paris, 77 Avenue Denfert Rochereau, 75014 PARIS, FRANCE

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Carlo Maria ZWÖLF, Observatoire de Paris, 61 Avenue de L'Observatoire, 75014 PARIS, FRANCE

Appendix 2: Meeting Agenda

Wednesday, 15 November 2023

14:00 – 14:30	Opening and introductions
14:30 – 15:45	VAMDC Nodes: status, updates and issues (~5 mins each)
15:45 – 16:00	Coffee Break
16:00 – 16:30	Discussion: procedures for handling new and expired databases

Thursday, 16 November 2023

14:00 – 14:30	XSAMS development, including extensions needed to the "case-by-case" schema for describing molecular states.
14:30 – 15:00	PyValem and related standards and libraries for the simplified description of atomic and molecular species, states, and processes: the future for adoption within VAMDC
15:00 – 15:30	**Marie-Lise DUBERNET**, *Paris Observatory, France* Issues with the VAMDC: A user's perspective
15:30 – 16:00	Giacomo MULAS, *Cagliari Observatory, Italy* XSAMS extensions for the PAH database
16:00 – 16:30	Discussion: outreach and educational activities

Friday, 17 November 2023

14:00 – 14:30	VAMDC Nodes: status, updates and issues (~5 mins each)
14:30 – 15:00	**Daan BOER**, *Eindhoven University of Technology, Netherlands* LXCat: A new data schema and web service
15:00 – 15:30	**Christian HILL**, *IAEA* CollisionDB and the PyValem library for atomic and molecular species and states
15:30 – 16:00	**Yaye AWA BA**, *Paris Observatory, France* VAMDC website: status and updates
16:00 – 16:30	**Thomas MARQUART**, *Uppsala University, Sweden* Applying Large Language Models to VAMDC
16:30 – 17:00	Discussion: Sustainability and future administration of the VAMDC

Appendix 3: VAMDC Board of Directors

The Board of Directors of the Virtual Atomic and Molecular Data Centres Consortium, as of November 2023 is given in the table below.

Name	*Database(s)*	*Notes*
Otoniel Denis Alpizar** *Universidad Autónoma de Chile, Santiago, Chile*	BASECOL	Confirmation pending
Vincent Boudon *Université de Bourgogne, Dijon, France*	*CaSDa	
Iouli Gordon *Harvard-Smithsonian Center for Astrophysics, Cambridge MA, USA*	HITRAN	Node not currently connected to VAMDC
Pierre Gratier *Laboratoire d'Astrophysique de Bordeaux, France*	KIDA	
Christian Hill* *International Atomic Energy Agency*	AMBDAS, [CollisionDB]	Co-Chair
Milan Dimitrijević *Astronomical Observatory of Belgrade, Serbia*	MolD, StarkB	
Christine Joblin *Institut de Recherche en Astrophysique et Planétologie (IRAP), Toulouse, France*	PAH	
Giuseppe Leto *Osservatorio Astrofisico di Catania, Italy*	LASP	
Bratislav Marinkovic *Institute of Physics Belgrade, Serbia*	BEAMDB, MOLD	
Nigel Mason *University of Kent, UK*	RADAM	
Tom Millar *Queen's University Belfast, UK*	UdfA	Note not currently connected
Giacomo Mulas *Osservatorio Astronomico di Cagliari. Italy*	PAH	
Izumi Murakami *Plasma Quantum Processes Unit, National Institute for Fusion Science, Japan*	NIFS	Note not currently connected
Nikolai Piskunov *Uppsala University, Sweden*	VALD3	
Yuri Ralchenko *National Institute of Standards and Technology, USA*	NIST-ASD	

Name	*Database(s)*	*Notes*
Tanya Ryabchikova *Institute of Astronomy of the Russian Academy of Sciences, Moscow, Russia*	VALD3	
Stephan Schlemmer* *Universität zu Köln, Germany*	CDMS	Co-Chair
Bernard Schmitt *Institut de planétologie et d'astrophysique de Grenoble (IPAG), France*	SSHADE, GhoSST	
Jonathan Tennyson *University College London, UK*	[ExoMol]	Note not currently connected
Vladimir Tyuterev *Université de Reims Champagne-Ardenne, France*	S&MPO	
Nicholas Walton *Institute of Astronomy, University of Cambridge, UK*	CHIANTI	
Carlo-Maria Zwölf *Observatoire de Paris, France*	TIPBASE / TOPBASE	
Duck-Hee Kwon *Korea Atomic Energy Research Institute (KAERI), Korea*	[PEARL]	Associated, non-voting member
Mi-Young Song *Korea Institute of Fusion Energy, Korea*	[KFE]	Associated, non-voting member
Charlotte Vastel *Institut pour la Recherche en Astrophysique et Planétologie, Toulouse, France*		VAMDC user

Appendix 4: VAMDC Scientific and Technical Board

The members of the Scientific and Technical Board of the Virtual Atomic and Molecular Data Centres Consortium, as of November 2023 is given in the table below.

Name
Damien Albert *Université Grenoble Alpes, France*
Otoniel Denis Alpizar *Universidad Autónoma de Chile, Santiago, Chile*
Yaye-Awa Ba *Observatoire de Paris, France*
Yurii Babikov *V. E. Zuev Institute of Atmospheric Optics, Tomsk, Russia*
Vincent Boudon *Université de Bourgogne, Dijon, France*
Franck Delahaye *Observatoire de Paris, France*
Marie-Lise Dubernet *Observatoire de Paris, France*
Masahiko Emoto *National Institute for Fusion Science, Japan*
Christian Endres *Max Planck Institute for Extraterrestrial Physics, Garching, Germany*
Alexander Fazliev *V. E. Zuev Institute of Atmospheric Optics, Tomsk, Russia*
Jean-Michel Glorian *Institut de Recherche en Astrophysique et Planétologie (IRAP), Toulouse, France*
Iouli Gordon *Harvard-Smithsonian Center for Astrophysics, Cambridge MA, USA*
Pierre Gratier *Laboratoire d'Astrophysique de Bordeaux, France*
Christian Hill *International Atomic Energy Agency*
Darko Jevremović *Astronomical Observatory of Belgrade, Serbia*
Roman Kochanov *V. E. Zuev Institute of Atmospheric Optics, Tomsk, Russia*
Duck-Hee Kwon *Korea Atomic Energy Research Institute (KAERI), Korea*
Giuseppe Leto *Osservatorio Astrofisico di Catania, Italy*
Peter Loboda *All-Russian Scientific Research Institute of Technical Physics (VNIITF), Snezhinsk, Russia*
Giuliano Malloci *Osservatorio Astronomico di Cagliari. Italy*

Name
Bratislav Marinković *Institute of Physics Belgrade, Serbia*
Thomas Marquart *Uppsala University, Sweden*
Tom Millar *Queen's University Belfast, UK*
Nicolas Moreau *Observatoire de Paris, France*
Giacomo Mulas *Osservatorio Astronomico di Cagliari. Italy*
Izumi Murakami *Plasma Quantum Processes Unit, National Institute for Fusion Science, Japan*
Yury Pakhomov *Institute of Astronomy of the Russian Academy of Sciences, Moscow, Russia*
Valery Perevalov *V. E. Zuev Institute of Atmospheric Optics, Tomsk, Russia*
Julien Penguen *Laboratoire d'Astrophysique de Bordeaux, France*
Nikolai Piskunov *Uppsala University, Sweden*
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Appendix 5: VAMDC Databases

This appendix lists details of the currently-active databases within the VAMDC Consortium.

AMBDAS: Atomic and Molecular Bibliographic Data System

The Atomic and Molecular Bibliographic Data System (AMBDAS) is a bibliographic database of literature on fundamental atomic and molecular processes for fusion applications maintained by the International Atomic Energy Agency.

URL: https://www-amdis.iaea.org/AMBDAS/

Host institution: International Atomic Energy Agency

Contact person: Christian HILL

Update status: Continuously updated.

Keywords: Atomic Spectroscopy; Collisional-Radiative Processes; Collisions in Plasmas; Electron – Ion Collisions; Electron – Molecule Collisions; Electronic Structure Calculations; Heavy Particle Collisions; Line Shapes; Plasma Diagnostics; Plasma Impurities; Plasma–Material Interaction; Tritium; Tungsten; Uncertainty Quantification

BASECOL

A database devoted to collisional ro-vibrational excitation of molecules by colliders including atoms, ions, molecules, and electrons.

URL: https://basecol.vamdc.eu/

Host institution: Paris Observatory (Observatoire de Paris)

Contact person: Marie-Lise DUBERNET

Update status: Continuously updated.

Keywords: Collisional-Radiative Processes; Collisions in Plasmas; Electron – Molecule Collisions

BEAMDB

Electron interaction cross sections for elastic scattering, electron excitation, ionization and total scattering.

URL: http://servo.aob.rs/emol/

Host institution: University of Belgrade

Contact person: Bratislav MARINKOVIĆ

Update status: Continuously updated.

Keywords: Collisional-Radiative Processes; Collisions in Plasmas; Electron – Ion Collisions; Electron – Molecule Collisions

CDMS: Cologne Database for Molecular Spectroscopy

The Cologne Database for Molecular Spectroscopy is a database of microwave spectroscopic data concerning 900+ species in the interstellar medium (ISM) and circumstellar envelopes.

URL: https://cdms.astro.uni-koeln.de/

Host institution: University of Cologne (Universität zu Köln)

Contact person: Stephan SCHLEMMER

Update status: Continuously updated (2–3 updates per month).

Keywords: Molecular Spectroscopy

CDSD: Carbon Dioxide Spectral Database

A high-temperature line list for CO_2, produced by the V.E. Zuev Institute of Atmospheric Optics, Tomsk Russia, in 2011: S. A. Tashkun and V. I. Perevalov, *Journal of Quantitative Spectroscopy and Radiative Transfer* **112**, 1403 (2011): https://doi.org/10.1016/j.jqsrt.2011.03.005.

URL: ftp://ftp.iao.ru/pub/CDSD-4000/

Host institution: V. E. Zuev Institute of Atmospheric Optics

Contact person: Valery PEREVALOV

Update status: Fixed at the 2011 version, but continues to be available at the IAO FTP site.

Keywords: Molecular Spectroscopy

CHIANTI

An atomic database for spectroscopic diagnostics of astrophysical plasmas. The supporting Python software library, ChiantiPy: https://github.com/chianti-atomic/ChiantiPy/ seems to be actively maintained.

URL: https://www.chiantidatabase.org/chianti_linelist.html

Host institution: Department of Applied Mathematics and Theoretical Physics (DAMTP), University of Cambridge

Contact person: Giulio DEL ZANNA

Update status: Last updated: 2015 (version 8.0).

Keywords: Astrophysics; Atomic Spectroscopy

ECaSDa, GeCaSDa, MeCaSDa, RuCaSDa, SHeCaSDa, TFMeCaSDa Calculated Spectroscopic Databases

A suite of "Calculated Spectroscopic Databases (CaSDa)" for the individual molecules: C_2H_4 (ECaSDa), GeH_4 (GeCaSDa), CH_4 (MeCaSDa), RuO_4 (RuCaSDa), SF_6 (SHeCaSDa), CF_4 (TFMeCaSDa).

URL: http://vamdc.icb.cnrs.fr/PHP/

Host institution: University of Burgundy (Université de Bourgogne)

Contact person: Vincent BOUDON

Update status: Updated as new calculations are completed.

Keywords: Molecular Spectroscopy

HITRAN: HIgh-resolution TRANsmission

HITRAN (HIgh-resolution TRANsmission) is a compilation of spectroscopic parameters that a variety of computer codes use to predict and simulate the transmission and emission of light in planetary atmospheres.

URL: https://hitran.org/

Host institution: Harvard-Smithsonian Center for Astrophysics (CfA)

Contact person: Iouli GORDON

Update status: Continuously updated, with major releases every four years.

Keywords: Molecular Spectroscopy

IDEADB

A database of cross sections for dissociative electron attachment to molecules.

URL: http://ideadb.uibk.ac.at/

Host institution: University of Innsbruck (Leopold-Franzens-Universität Innsbruck)

Contact person: Felix DUENSING

Update status: Apparently no longer updated, but the web service is still useable.

Keywords: Collisional-Radiative Processes; Collisions in Plasmas; Electron – Molecule Collisions

KIDA: The Kinetic Database for Astrochemistry

The Kinetic Database for Astrochemistry is a database of kinetic data of interest for astrochemical (interstellar medium and planetary atmospheres) studies.

URL: http://kida.astrophy.u-bordeaux.fr/

Host institution: Laboratoire d'Astrophysique de Bordeaux

Contact person: Pierre GRATIER

Update status: Continuously updated.

Keywords: Astrophysics

LASp

Transmission and optical depth data of water ice experiments are available for the temperature range from 12.5 to 150 K. The database also includes optical constants of solid state CO, CO_2, and CH_4 deposited at various temperatures.

URL: http://web.ct.astro.it/weblab/dbindex.html#dbindex

Host institution: Osservatorio Astrofisico di Catania

Contact person: Giuseppe Leto

Update status: Continuously updated.

Keywords: Solid Spectroscopy; Astrophysics

MolD

A database of photodissociation cross sections with an interactive interface, run by the Institute of Physics Belgrade and Astronomical Observatory Belgrade.

URL: http://servo.aob.rs/mold/

Host institution: University of Belgrade

Contact person: Vladimir Srećković

Update status: Continuously updated.

Keywords: Astrophysics; Molecular Spectroscopy

NIFS Databases

A suite of databases of fundamental atomic and molecular data for fusion applications developed and maintained by the Atomic and Molecular Research Center at the National Institute for Fusion Science, Japan.

URL: https://dbshino.nifs.ac.jp/nifsdb/

Host institution: Plasma Quantum Processes Unit, National Institute for Fusion Science (NIFS)

Contact person: MURAKAMI Izumi

Update status: Continuously updated.

Keywords: Atomic Spectroscopy; Collisional-Radiative Processes; Collisions in Plasmas; Electron – Ion Collisions; Electron – Molecule Collisions; Fusion; Plasma Diagnostics

NIST Atomic Spectra Database (ASD)

A database of radiative transitions and energy levels in atoms and atomic ions managed by the US National Institute of Standards and Technology.

URL: https://physics.nist.gov/PhysRefData/ASD/lines_form.html

Host institution: National Institute of Standards and Technology (NIST)

Contact person: Yuri RALCHENKO

Update status: Continuously updated.

Keywords: Atomic Spectroscopy; Electronic Structure Calculations

PAH: Properties of Polyaromatic Hydrocarbons

Database of theoretical spectra of polyaromatic hydrocarbons and pure carbon clusters.

URL: https://www.dsf.unica.it/~gmalloci/pahs/

Host institution: Observatory of Cagliari, Italy

Contact person: Giuliano Malloci

Update status: Continuously updated.

Keywords: Molecular Spectroscopy; Astrophysics

PEARL: Photonic Electronic Atomic Reaction Library

The Photonic Electronic Atomic Reaction Library (PEARL) is a database of photoionization/ electron-impact ionization and dielectronic recombination cross sections and rate coefficients maintaned by the Atomic Data Center of the Korea Atomic Energy Research Institute (KAERI).

URL: http://pearl.kaeri.re.kr/pearl/

Host institution: Korea Atomic Energy Research Institute (KAERI)

Contact person: Duck-Hee KWON

Update status: Continuously updated.

Keywords: Atomic Spectroscopy; Collisional-Radiative Processes; Collisions in Plasmas; Electron – Ion Collisions; Electron – Molecule Collisions; Electronic Structure Calculations

S&MPO (Spectroscopy and Molecular Properties of Ozone)

A database of theoretical and experimentally-derived spectroscopic and molecular properties of ozone jointly developed by Groupe de Spectrométrie Moléculaire et Atmosphérique (GSMA) and the V.E. Zuev Institute of Atmospheric Optics (Tomsk, Russian Academy of Sciences).

URL: https://smpo.univ-reims.fr/

Host institution: University of Reims, France

Contact person: Vladimir TYUTEREV

Update status: Continuously updated.

Keywords: Molecular Spectroscopy

SESAM (SpEctroScopy of Atoms and Molecules)

A molecular spectroscopy database dedicated to electronic spectra of diatomic molecules.

URL: https://sesam.obspm.fr/

Host institution: Paris Observatory, France

Contact person: Nicolas MOREAU

Update status: Continuously updated.

Keywords: Molecular Spectroscopy

SPECTR-W3

A database of spectroscopic properties of atoms and ions, including ionization potentials, energy levels, transition frequencies and intensities, and collisional data). Managed by the Joint Institute for High Temperatures (JIHT) of the Russian Academy of Sciences (RAS) and the All-Russian Scientific Research Institute Of Technical Physics (VNIITF).

URL: http://spectr-w3.snz.ru/index.phtml

Host institution: All-Russian Scientific Research Institute of Technical Physics (VNIITF)

Contact person: Peter LOBODA

Update status: Last updated: since January 2014.

Keywords: Atomic Spectroscopy; Collisional-Radiative Processes; Collisions in Plasmas; Electron – Ion Collisions; Electron – Molecule Collisions; Electronic Structure Calculations; Heavy Particle Collisions; Molecular Spectroscopy

SSHADE

SSHADE provides various types of spectral data (mostly in X-, UV-, Vis-, IR- and sub-mm ranges) for a wide range of solids, including ices, minerals, organics, extraterrestrial samples.

URL: https://www.sshade.eu/doi/10.26302/SSHADE

Host institution: Institut de planétologie et d'astrophysique de Grenoble (IPAG), France

Contact person: Bernard SCHMITT

Update status: Continuously updated.

Keywords: Solid Spectroscopy; Astrophysics

STARK-B: Stark-Broadening

A database for "Stark" broadening of isolated lines of atoms and ions in the impact approximation.

URL: https://stark-b.obspm.fr/

Host institution: Paris Observatory (Observatoire de Paris)

Contact person: Sylvie SAHAL-BRÉCHOT

Update status: Continuously updated.

Keywords: Atomic Spectroscopy; Collisions in Plasmas; Line Shapes

TipTopbase

Two databases: TIPbase, containing fine-structure atomic data computed for ions of astrophysical interest; and TOPbase, an online atomic database created as part of the [Opacity Project](http://cdsweb.u-strasbg.fr/topbase/publi.html).

URL: https://tiptopbase.obspm.fr/

Host institution: Paris Observatory (Observatoire de Paris)

Contact person: Claudio MENDOZA

Update status: Last updated: although the database itself may not have been updated for some time (2009?), the data service itself continues to run effectively.

Keywords: Astrophysics; Atomic Spectroscopy

UMIST RATE2012 (UdfA)

The UMIST Database for Astrochemistry contains reaction rate coefficient data for species of astrophysical interest, with a particular emphasis on hydrocarbons and their ions.

URL: http://udfa.ajmarkwick.net/

Host institution: University of Manchester

Contact person: Tom MILLAR

Update status: Last updated: 2012; new release due in 2024.

Keywords: Astrophysics; Low Temperature Plasmas

VALD: Vienna Atomic Line Database

The Vienna Atomic Line Database (VALD) is a collection of atomic and molecular transition parameters of astronomical interest. Now identifying as VALD3, it is provided by mirrored servers in Uppsala, Sweden, Vienna, Austria, and Moscow, Russia.

URL: http://vald.astro.uu.se/

Host institution: Uppsala University

Contact person: Nikolai PISKUNOV

Update status: Continuously updated.

Keywords: Astrophysics; Atomic Spectroscopy; Molecular Spectroscopy

W@DIS (Water Information System)

The W@DIS information system is designed to provide access to data, information, and ontologies relating to the quantitative spectroscopy of water required for solving fundamental and applied problems pertaining to a number of subject domains, including atmospheric optics and astronomy.

URL: https://wadis.saga.iao.ru/

Host institution: V. E. Zuev Institute of Atmospheric Optics, Tomsk, Russia

Contact person: Alexander Fazliev

Update status: Continuously updated.

Keywords: Molecular Spectroscopy

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