Atomic and Molecular Data in Astrophysics
IAU and VAMDC

M.L. Dubernet

LERMA, Observatory of Paris, PSL University, CNRS

France

marie-lise.dubernet@observatoiredeparis.psl.eu

Disclaimer :
Any error in describing the material provided by my colleagues is only mine.
Any mistake in presenting materials describing official french institutions is only mine.

Current Responsabilities : Chair of VAMDC consortium and Vice-President of IAU B5 Commission

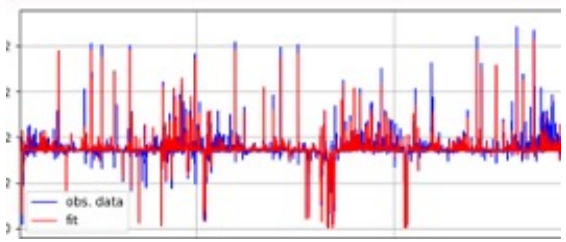
Why Atomic and Molecular Data in Astrophysics ?

Atoms and Molecules emit/absorb electromagnetic radiation → Stars, Comets, Solar Planets, ExoPlanets, Interstellar Medium

Different local conditions :

- Temperature and density, Different Species
- Different type de wavelengths
- Different types of processes such collisional excitation, reaction, photodissociation, etc

Astronomical Observations
mm, submm (ALMA, ..)
IR (JWST, ..)
UV (LUVOIR, ..)
Optical (ELT, VLTI, ..)
X (CHANDRA, ATHENA,..)



Astrophysical Spectra
(or images)

Analysis of Observed Spectra : models object, radiative transfer methods
atomic and molecular processes <-> A&M Data

Modelisation of the Objects
physical model of the object
atomic and molecular processes <-> A&M Data

Issues with atomic and molecular data
- lack of existing data for many processes
- problems with accuracy of the A&M data

- easy access to the A&M data
- tracability of the A&M data

Lab. Astro Challenges

Need for new experiments
Need for new calculations

Lab. Astro. Data

Databases
Distribution of A&M data
Good Practices with management of A&M data
Interfaces with astro tools and astro codes

Table 1: Molecules detected in AGB CSEs

2-atoms:	AlCl	CP	NaCl	SiN
	AlF	CS	OH	SiO
	AlO	ClH	PN	SiS
	C_2	FH	PO	SO
	CO	KCl	SiC	TiO
	CN			
3-atoms:	AlOH	CO_2	H_2S	c-SiC_2
	AlNC	CaNC	HNC	SiCN
	C_3	FeCN	KCN	SiCSi
	C_2H	HCN	MgCN	SiNC
	C_2N	HCP	MgNC	SO_2
	C_2P	H_2O	NaCN	TiO_2
	C_2S			
4-atoms:	c-C_3H	C_3S	H_2CS	NH_3
	ℓ-C_3H	C_2H_2	HMgNC	PH_3
	C_3N	HC_2N	MgC_2H	c-SiC_3
	C_3O	H_2CO	NC_2P (?)	
5-atoms:	C_5	CH_2CN	HC_3N	HNC_3
	C_4H	CH_4	HC_2NC	MgC_3N
	C_4Si	CH_2NH	H_2C_3	SiH_4
	c-C_3H_2			
6-atoms:	C_5H	C_4H_2	HC_4N	MgC_4H
	C_5N	C_2H_4	H_2C_4	SiH_3CN
	C_5S	CH_3CN		
≥7-atoms:	C_6H	CH_2CHCN	HC_5N	H_2C_6
	C_7H	CH_3CCH	HC_7N	
	C_8H	CH_3SiH_3	HC_9N	
Ions:	C_4H^-	C_6H^-	C_8H^-	HCO^+
	CN^-	C_3N^-	C_5N^-	


OUT OF THIS WORLD

A wealth of molecules is found in interstellar clouds

2 atoms: H_2, AlF, AlCl, C_2, CH, CH^+, CN, CO, CO^+, CP, CSi, HCl, KCl, NH, NO, NS, NaCl, OH, PN, SO, SO^+, SiN, SiO, SiS, CS, HF, SH, FeO

3 atoms: C_3, C_2H, C_2O, C_2S, CH_2, HCN, HCO, HCO^+, HCS^+, HOC^+, H_2O, H_2S, HNC, HNO, MgCN, MgNC, N_2H^+, N_2O, NaCN, OCS, SO_2, c-SiC_2, CO_2, NH_2, H_3^+, SiCN, AlNC

4 atoms: c-C_3H, l-C_3H, C_3N, C_3O, C_3S, C_2H_2, HCCN, $HCNH^+$, HNCO, HNCS, $HOCO^+$, H_2CO, H_2CN, H_2CS, H_3O^+, NH_3, SiC_3

5 atoms: C_5, C_4H, C_4Si, l-C_3H_2, c-C_3H_2, CH_2CN, CH_4, HC_3N, HC_2NC, HCOOH, H_2CHN, H_2C_2O, H_2NCN, HNC_3, SiH_4, H_2COH^+

6 atoms: C_5H, l-H_2C_4, C_2H_4, CH_3CN, CH_3NC, CH_3OH, CH_3SH, HC_3NH^+, HC_2CHO, NH_2CHO, C_5N

7 atoms: C_6H, CH_2CHCN, CH_3C_2H, HC_5N, $HCOCH_3$, NH_2CH_3, c-C_2H_4O, CH_2CHOH

8 atoms: CH_3C_3N, $HCOOCH_3$, CH_3COOH, C_7H, CH_2OHCHO

9 atoms: CH_3C_4H, CH_3CH_2CN, $(CH_3)_2O$, CH_3CH_2OH, HC_7N, C_8H

10 atoms: CH_3C_5N, $(CH_3)_2CO$, NH_2CH_2COOH

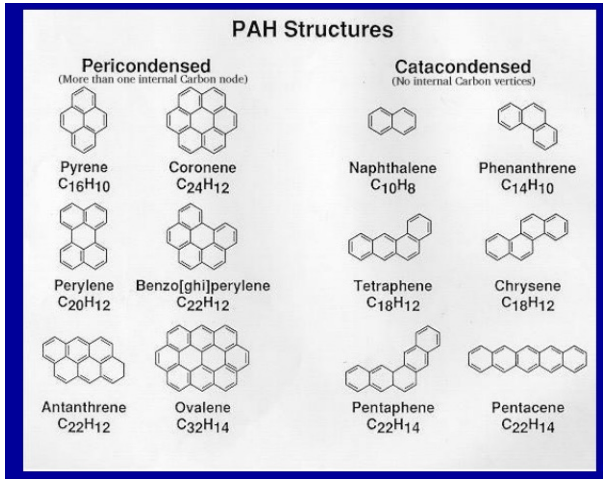
11 atoms: HC_9N

13 atoms: $HC_{11}N$

NOTE: Evidence suggests that much larger molecules such as polycyclic aromatic hydrocarbons and fullerenes are also present.

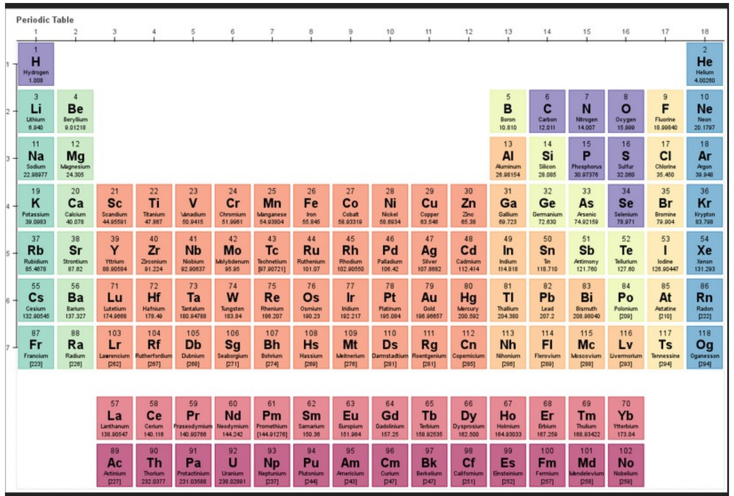
SOURCE: National Radio Astronomy Observatory

Interstellar Medium



How are they formed : gaz phase, on the surface of grains ?

Some examples



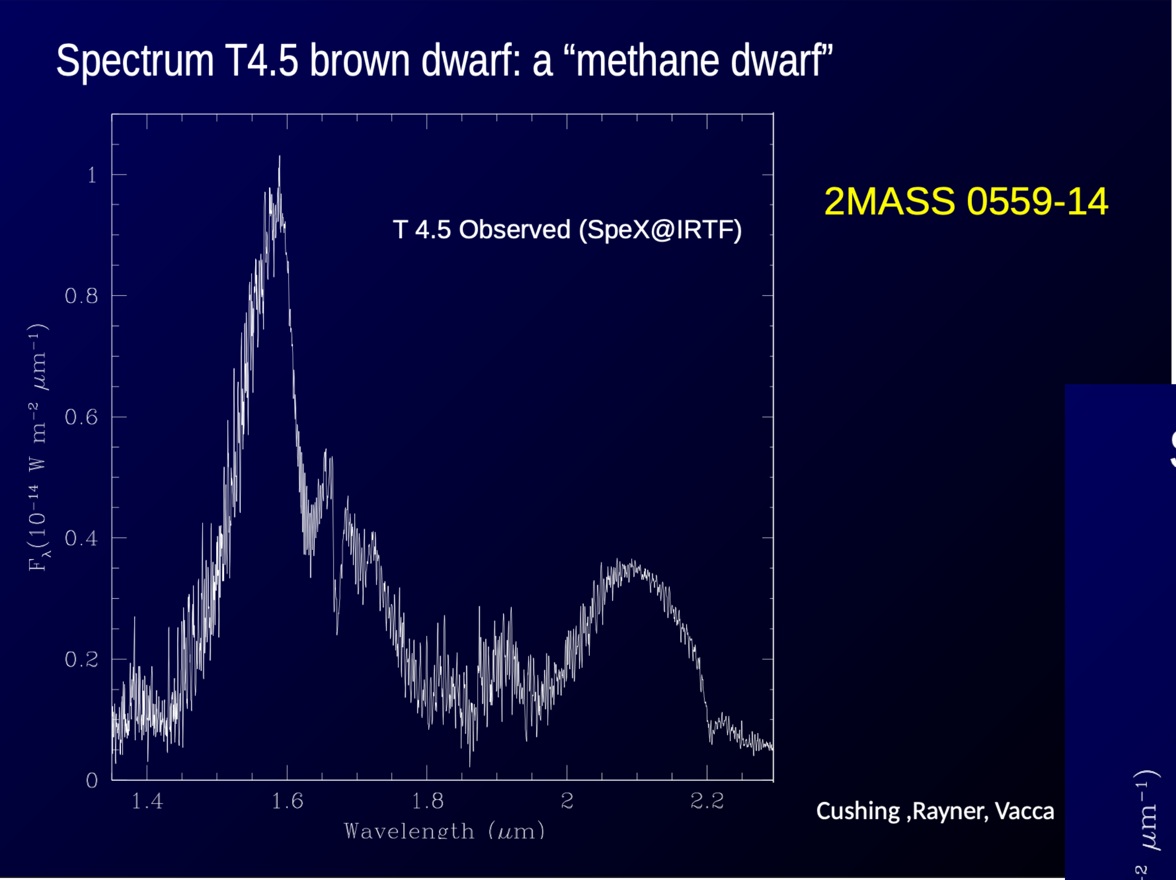
Study of (exo) planets and small objects : what the physical, chemical, dynamical processes underlying the evolution of thoses objects ?

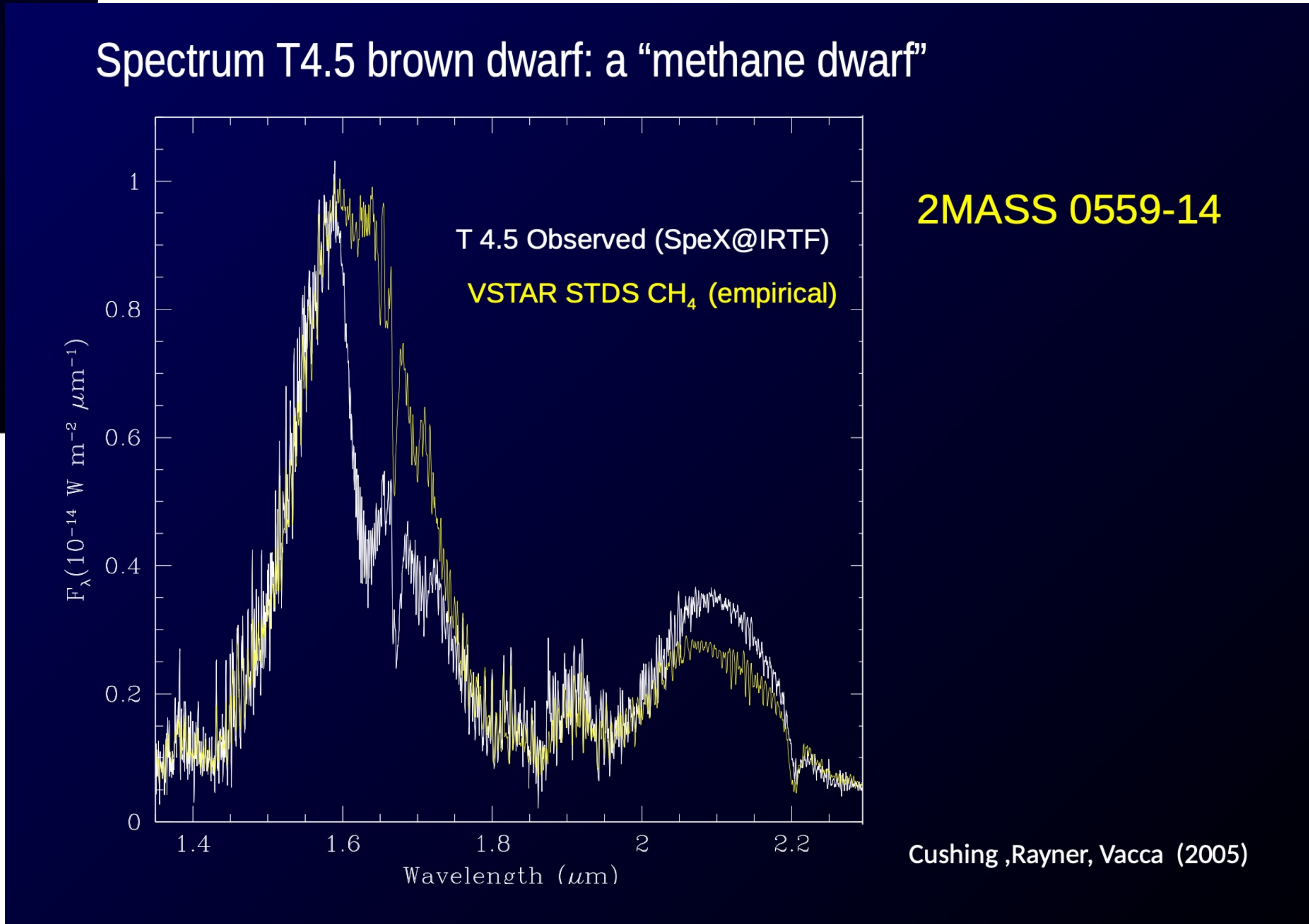
Stellar environnement : what are the key parameters in the interaction between stars, disks, exoplanets ?

Solar Environnements and plasmas

Exemple of how knowledge on astrophysical object progresses thanks to new calculations that provide more data

Here is the status in 2005





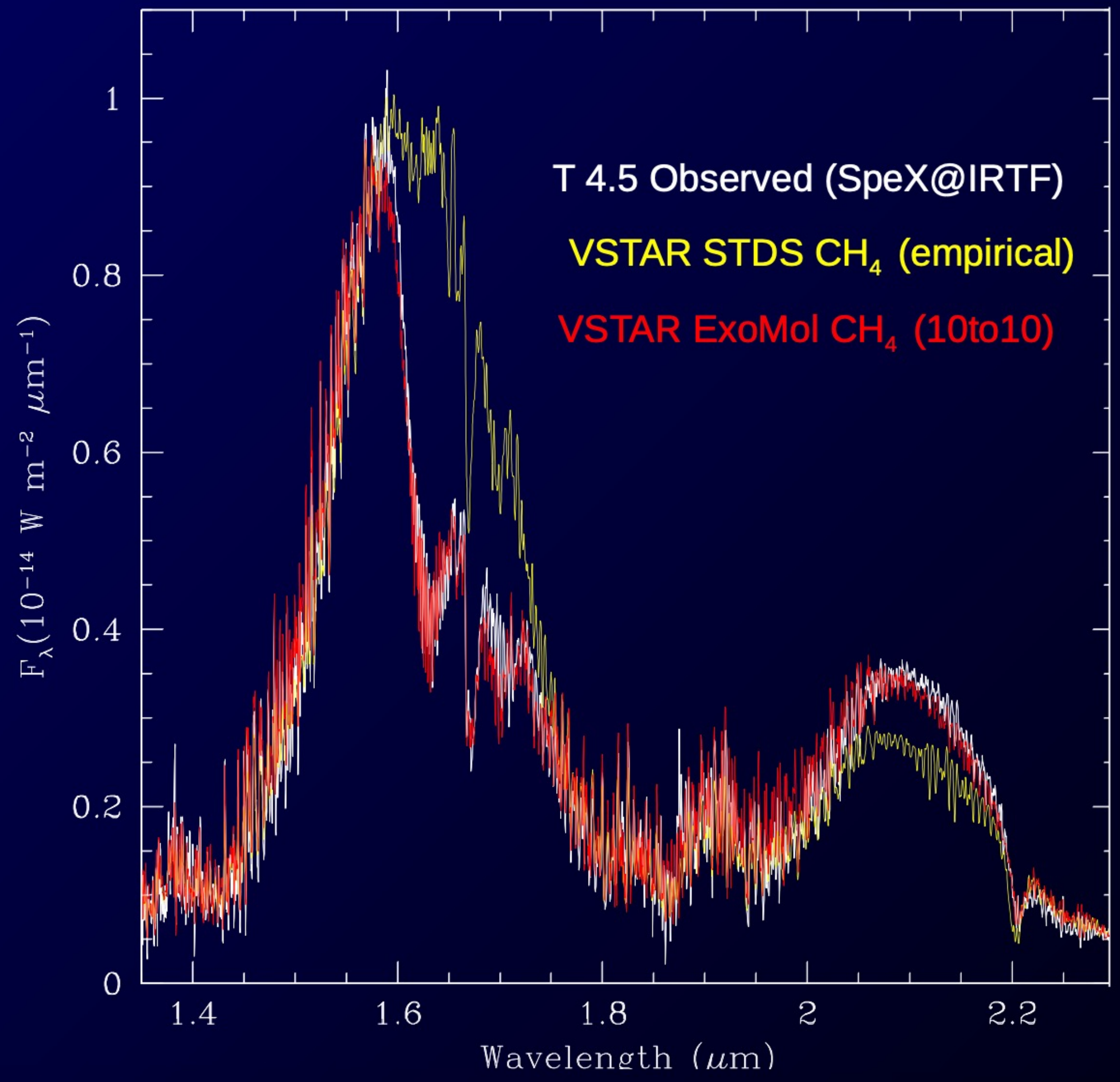
Courtesy of J. Tennyson

9 years later
With the ExoMol Data
On CH_4 (200 times
more data then previously
- High Temperature)

It takes effort = grant
and time to obtain
those new indispensable
molecular data

Courtesy of J. Tennyson

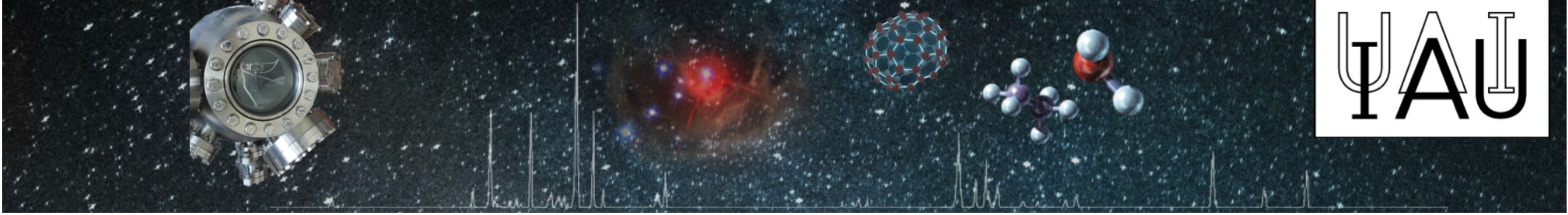
Spectrum T4.5 brown dwarf: a "methane dwarf"



2MASS 0559-14

SN Yurchenko, J Tennyson, J Bailey, MDJ Hollis, G Tinetti, PNAS, 111, 9379 (2014)

Cushing ,Rayner, Vacca (2005)



B5 IAU Commission (since 2015)

General Purpose of the B5 commission (Presidents : F. Salama, H. Fraser, P. Barklem)

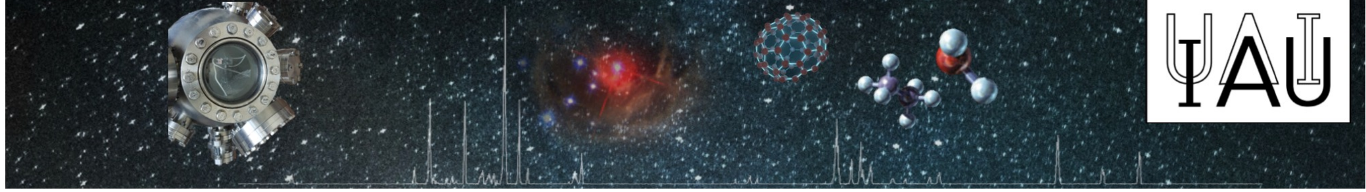
https://www.iau.org/science/scientific_bodies/commissions/B5/

B5-B2 working Group on “Lab. Astro Data”

https://www.iau.org/science/scientific_bodies/working_groups/335/

IAU GA B5 commission days, 8th August 2022

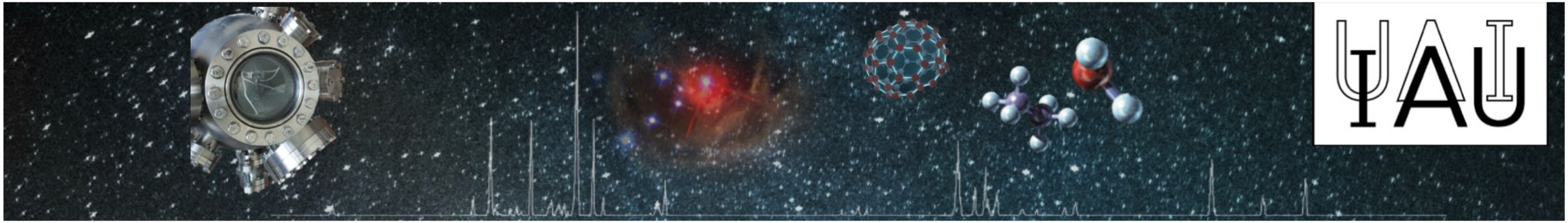
https://www.iauga2022.org/program/program_05_2.asp?sMenu=abo5



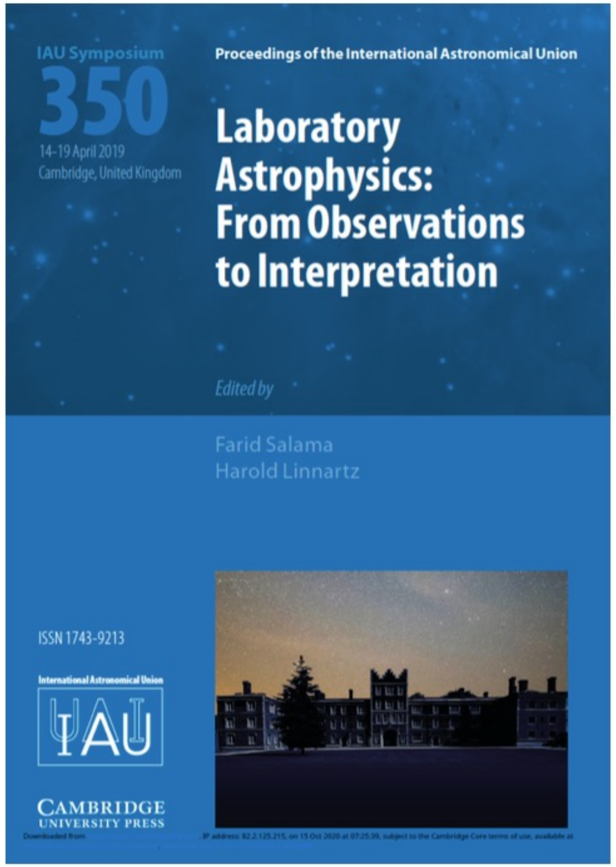
B5 IAU commission

- Address the multidisciplinary needs and requirements of modern astronomy and planetary science.
- Commission B5 is a strongly cross-disciplinary commission with the aim to assist IAU members in providing the data needed to interpret and understand astronomical observations and to promote Laboratory Astrophysics.
- The Commission encompasses the 4 fundamental research areas :
  - atomic and molecular astrophysics → 1 WG on molecular spectroscopy
  - dust and ices
  - plasma astrophysics
  - nuclear and particle astrophysics
- 1 WG on Lab. Astro. Data
- The interdisciplinary studies include experiment, theory, and modeling, from the nuclear and atomic/molecular level to application on astronomical scales.

Courtesy F. Salama, ECLA Conference 2021



Activities of Commission B5



- Advise IAU on Laboratory Astrophysics
- Promote Laboratory Astrophysics
- Organize Meetings (2018 GA, 2019 non-GA Symposium*)
- Establish Working Groups* to undertake well-defined tasks for limited time periods on behalf of the Commission as a whole
- Run Elections
- Yearly evaluation of IAU Symposium proposals
- Report to IAU*:
  - Annual and Triennial Reports of Commission activities
  - Annual and Triennial Reports of Working Groups

Courtesy F. Salama, ECLA Conference 2021

Inter-Commission B2-B5 WG

“Laboratory Astrophysics Data Compilation, Validation and Standardisation: from the Laboratory to FAIR Usage in the Astronomical Community”

- Objectives : provide a platform where to discuss the FAIR usage of laboratory astrophysics data in astronomy and astrophysics (Findability, Accessibility, Interoperability, Reuse).
- Timing :
  - Year 1 : to provide a state-of-the-art report on the existing infrastructures and databases
  - Year 2 : to identify the bottlenecks in providing the data (via publications, databases, infrastructure) to the astronomical community and in the FAIR usage of the laboratory astrophysics data by the astronomical community
  - Year 3 : to provide practical and political recommendations related to optimizing the process from laboratory data to astrophysics and vice-versa

IAU General Assembly, Busan 2022
Division B session on the 8th August

- Morning : 10.45 - 12.15 Session 2A: Laboratory Astrophysics commission meeting (Chair : Paul Barklem)
  - CB5 - Laboratory Astrophysics - present and future (Paul Barklem)
  - Spectroscopic and Radiative Data for Molecules (TbD)
- **Regional Lab. Astrop. Reports:**
  - Korea (Dongsu Ryu)
  - South America/Brazil (Beatriz Barbuy)
  - Middle East/Egypt (Osama M.A. Shalabiea)
  - South East Asia/Singapore (Peng Kian Tan)
  - China (Jiayong Zhong)
  - Japan (Naoki Watanabe)
- Conclusion and discussion (Paul Barklem)

IAU General Assembly, Busan 2022 Division B session on the 8th August

- Afternoon : 13.30 – 15.00 Session 3A: Laboratory Astrophysics Databases: from the provider to the user: encouraging FAIRness (Chair : ML Dubernet and B. Berriman)
- WG Activities and Plans (ML Dubernet)
- FAIR principles in VAMDC (ML Dubernet)
- FAIR principles in IVOA (B. Berriman)
- PAH community (Christiaan Boersma - NASA ARC/SJSU, USA)
- Dust/Ice community (Cornelia Jägger - MPI & Frederich Schiller Univ., Germany)
- Planetology : How do people get organized with respect to access to A&M&Solids data for missions (Miriam Rengel, MPI für Sonnensystemforschung, Göttinger, Germany)
- Examples of astro analysis tools: ENIIGMA, Will Rocha (Leiden University, Nederthlands)
- General Discussion and concluding remarks

Example of the WG on-going work : State-of-the-art

- Make List of Codes and Tools using a questionnaire …
- List of Databases / Infrastructure known to provide data to the astrophysical community using a questionnaire …
- List of "Virtual Research Environment" that are available and could be used by the Lab Astro Community
- List of initiatives linked to standards to describe atomic, molecular, solid data for Lab Astrophysics Data.

You are most welcome to be a member of and/or participate to the IAU WG

Just contact me : marie-lise.dubernet@observatoiredeparis.psl.eu

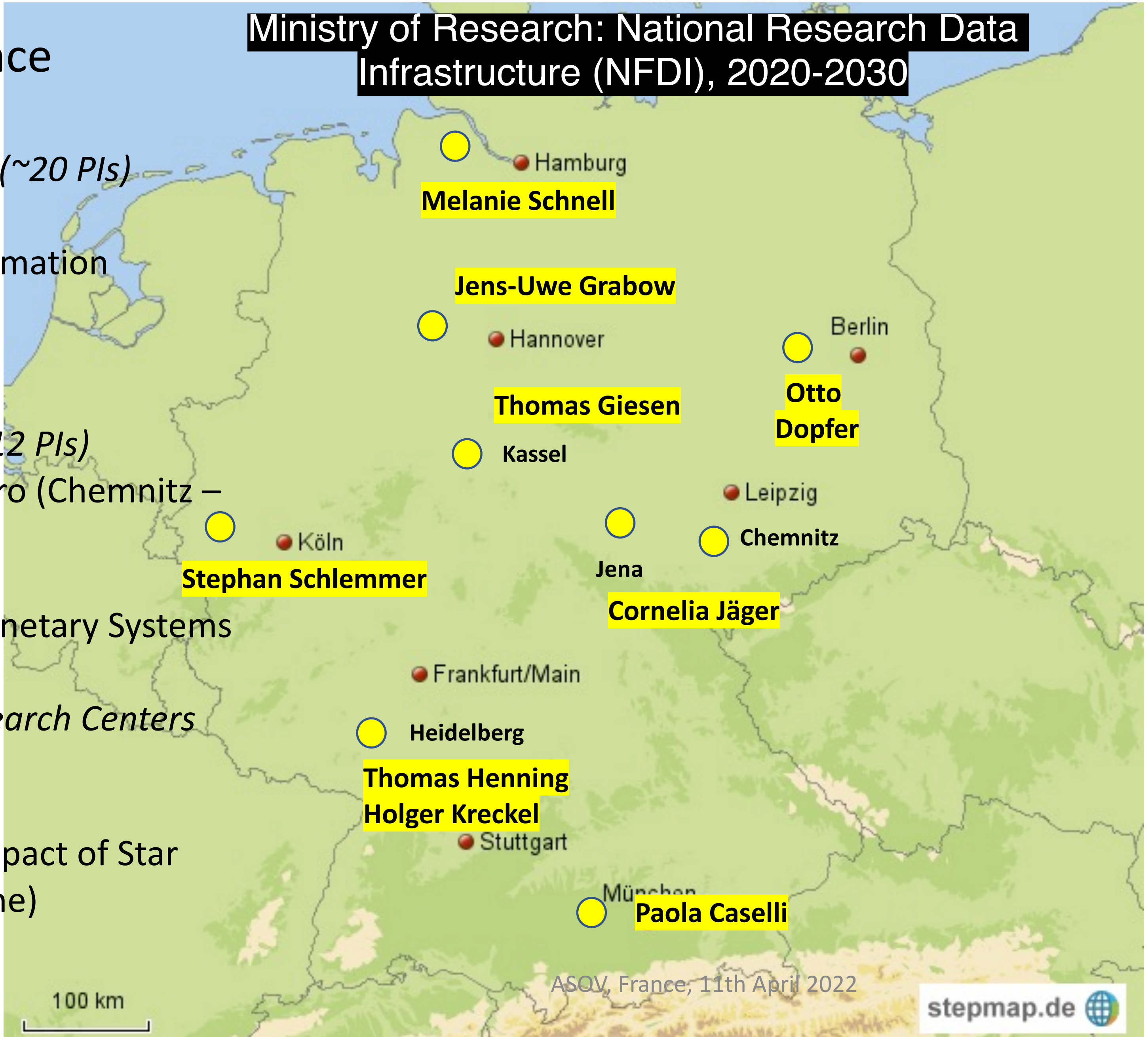
We are interested about the political/organisational context of each country-region

Context of Germany

Provided by Prof. Stephan Schlemmer (Cologne University)

Laboratory Astrophysics Family in Germany

Ministry of Research: National Research Data Infrastructure (NFDI), 2020-2030



German Science Foundation:

Priority Programs (~20 PIs)

1995 - 2001
Physics of Star Formation
2012-2017
Physics of the ISM

Research Units (~12 PIs)

1999-2005 Labastro (Chemnitz – Jena)
2017-2023
Debris Disks in Planetary Systems

Collaborative Research Centers (~15PIs)

2011- 2022
Conditions and Impact of Star Formation (Cologne)

More than
20 years of collaboration

Continued annual workshops

2020: 8 groups

Participation in collaborative research supported by German Science Foundation (DFG)

FOR DATA Management Context :
Context of Research Data Alliance
FAIR Principles

- RDA : https://www.rd-alliance.org/
  - Working Groups that deliver recommendations concerning various aspects of data management but also concerning codes
  - Bi-Annual Conference : Next one June 2022, Seoul (with the Data Week)
- FAIR Principles : https://www.go-fair.org/fair-principles/
- IVOA context
- All database, infrastructure and user software/codes should follow the FAIR principles in order for science to be reproducible and trusted.

A few Databases and Thematic Portals

LIDA DB : provided by H. Linnartz

NASA Ames PAH, Cosmic PAH, ExoMol Databse : snapshots

Astrochem-tools : provided by V. Wakelam

Opacity Project : provided by F. Delahaye

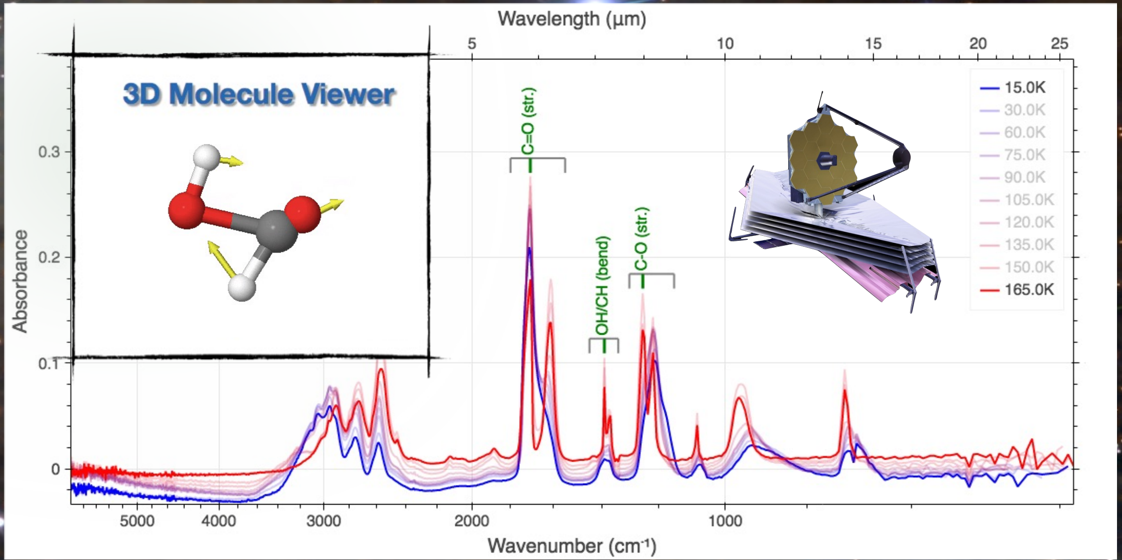
ExoMol : provided by J. Tennyson

LIDA [Leiden Ice Database for Astrochemistry]
icedb.strw.leidenuniv.nl

Details available soon from Rocha et al. (2022)

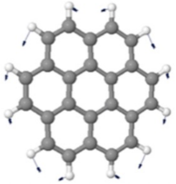
Example:
IR spectrum:
HCOOH:

JWST/ERS
ICE AGE



1068 different spectra; different compositions; different mixing ratios; range of astrophysically relevant temperatures; analytical tools, for assignments and spectral simulations

Designed to fully support JWST ice observations



The NASA Ames PAH IR Spectroscopic Database (PAHdb)

https://www.nasa.gov/ames/spacescience-and-astrobiology/the-nasa-ames-pah-ir-spectroscopic-database-pahdb)

Database and Tools

Presentation at IAU GA 2022, Busan

Documentation Portal

NASA Ames PAH IR Spectroscopic Database

Welcome to the NASA Ames PAH IR Spectroscopic Database Documentation Portal. More information about the NASA Ames PAH IR Spectroscopic Database (PAHdb) can be found at the PAHdb website. Below you can access the website documentation, documentation describing the different software Application Programming Interfaces (APIs) and a cookbook with recipes for using the (software) tools.

Website Manual

website

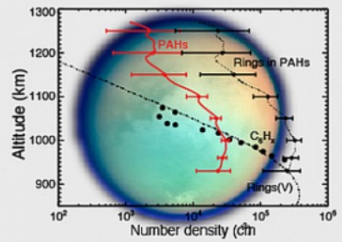
AmesPAHdbIDLSuite | *AmesPAHdbPythonSuite* | *pyPAHdb*

repository | repository | repository

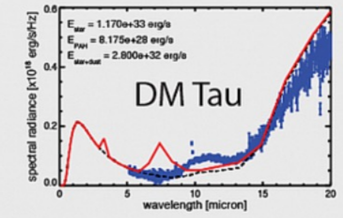
Cookbook

The NASA Ames PAH IR Spectroscopic Database is being supported through a directed Work Package at NASA Ames titled: "Laboratory Astrophysics – The NASA Ames PAH IR Spectroscopic Database".

France, 11th

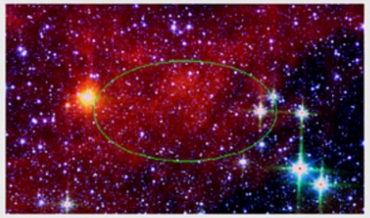


Solar System

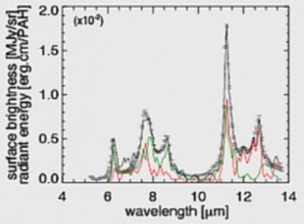


Disks

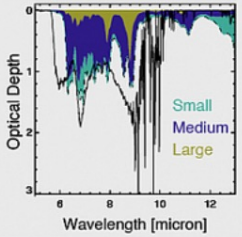
Novae



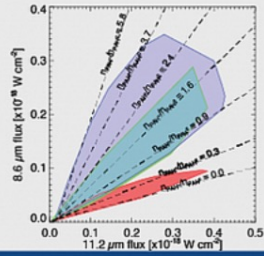
Globules



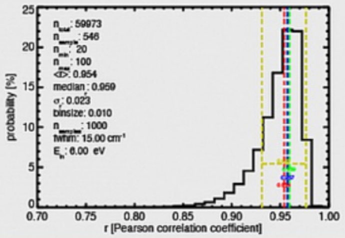
Galaxies



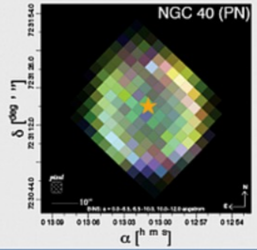
Ices



Proxy Calibration



Universal Nature



Nebulae

Log In

Search | Search

Recent Changes Media Manager Sitemap

Cosmic PAH portal

News Activities Platforms Production Databases Tools Teams

http://cosmic-pah.irap.omp.eu

Table of Contents

COSMIC PAH portal

Description

Polycyclic aromatic hydrocarbons (PAHs) and related molecular species (e.g. fullerenes) are key species in astrophysical environments. The primary objective of the Cosmic PAH portal is to ease access to databases and tools in order to:

- **Identify** these species in astrophysical environments and in extraterrestrial samples.
- **Understand** their formation pathways and their link with related molecular species such as carbon clusters and fullerenes.
- **Model** their evolution in astrophysical environments and their impact on the physical and chemical conditions.

Link content

- **Molecular databases** developed by the team, both theoretical and experimental.
- **Simulated spectra databases** for PAH infrared emission in various astrophysical environments.
- **Spectral analysis tools** to analyze in a consistent way spectra from experiments. theoretical calculations, and astrophysical observations.
- **Tools to model spectra** in astrophysical environments using experimental and theoretical data.

erc

irap astrophysique & planétologie

OBSERVATOIRE VIRTUEL GRAND SUD OUEST

cnrs dépasser les frontières

cnes CENTRE NATIONAL D'ÉTUDES SPATIALES

OAC Osservatorio Astronomico di Cagliari

INAF

Astrochem-tools

(https://astrochem-tools.org/)

Services developed and maintained at the Observatoire Aquitain des Sciences de l'Univers (OASU) and the Laboratoire d'astrophysique de Bordeaux (LAB) for the astrochemical community.

KIDA

KInetic Database for Astrochemistry
http://kida.astrochem-tools.org/

ISA

InterStellar Abundance database
http://isa.astrochem-tools.org/

ACN

AstroChemical Newsletter
http://acn.astrochem-tools.org/

Nautilus

Nautilus gas-grain code
https://forge.oasu.u-bordeaux.fr/LAB/astrochem-tools/pnautilus

Astrochemical Forum

Astrochemical forum
https://discourse.astrochem-tools.org/

Coordinators: Pierre Gratier and Valentine Wakelam

KIDA
KINETIC DATABASE FOR ASTROCHEMISTRY

Funding

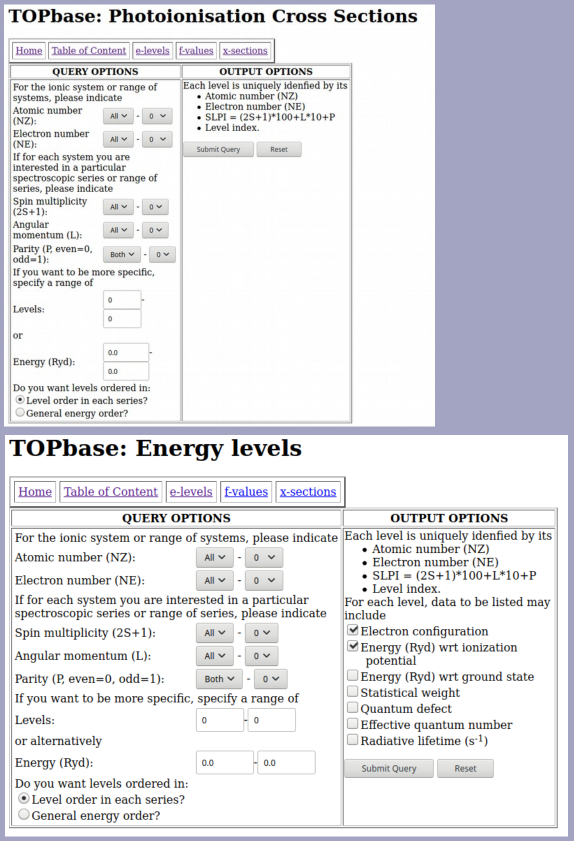
erc
Agence Nationale de la Recherche ANR
Observatoire aquitain des sciences de l'univers OASU
cnrs
université de BORDEAUX
pcmi
LAB
VAMDC consortium

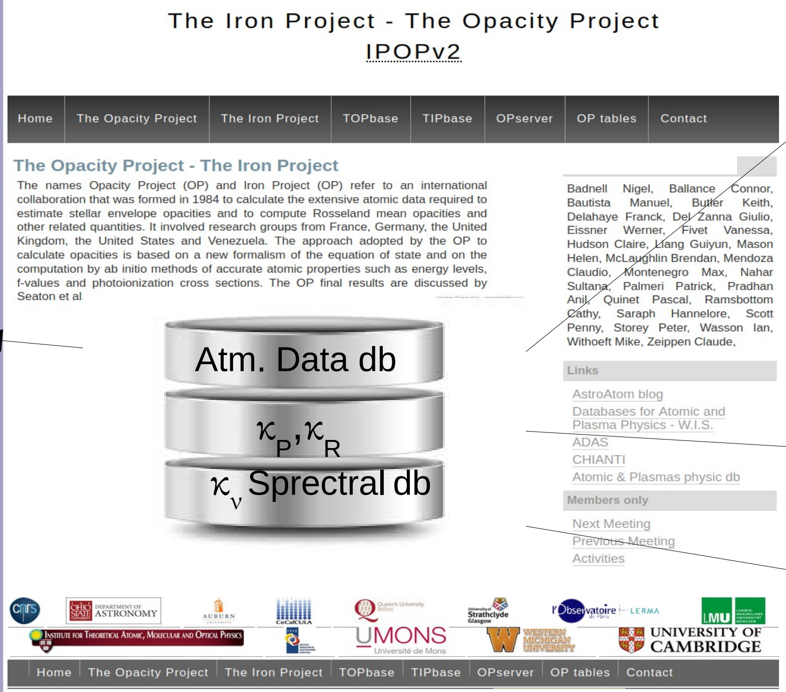
Stellar

The Opacity Project: Opacitiy services

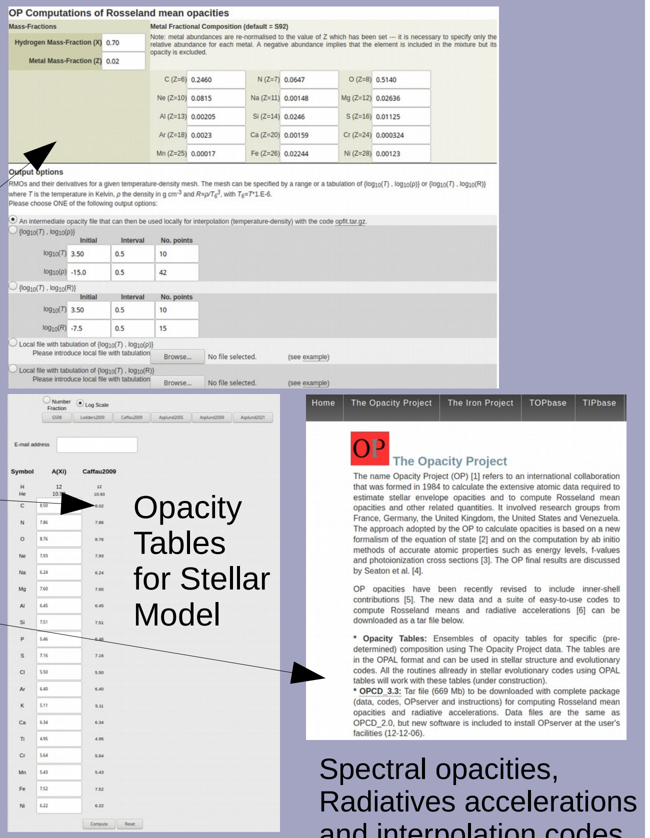
https://opserver.obspm.fr/

Raw atomic data





Opacities



Spectral opacities, Radiatives accelerations and interpolation codes

Next: Experimental measurements!

ExoMol

Molecular line lists for exoplanet and other atmospheres

Jonathan Tennyson and Sergey Yurchenko (UCL),

Hot line lists; Published in MNRAS

I. BeH, MgH, CaH
II. SiO
III. HCN/HNC
IV. CH_4
V. NaCl, KCl
VI.PN
VII. PH_3
VIII. H_2CO
IX. AlO
X. NaH
XI. HNO_3
XII. CS
XIII. CaO
XIV. SO_2
XV. HOOH
XVI. H_2S
XVII. SO_3
XVIII. VO
XIX. $H_2{}^{18}O$, $H_2{}^{17}O$
XX. H_3^+

XXI. NO
XXII. SiH_4
XXIII. PO, PS
XXIV. SiH
XXV. SiS
XXVI. SN, SH
XXVII. AlH
XXVIII. C_2H_4
XXIX. CH_3Cl
XXX. $H_2{}^{16}O$
XXXI. C_2
XXXII. TiO
XXXIII. MgO

XXXIV. PH
XXXV. NH_3
XXXVI SH (UV)
XXXVII HCCH
XXXVIII SiO_2
XXXIX CO_2
XL. H_3O^+
XLI. NaOH, KaOH
XLII. NO (UV)
XLIII. NaO
XLIV. SiO (UV)
XLV. MgH, CaH (UV)

Formal data releases:
J. Tennyson *et al.*, J. Mol. Spectrosc. **373**, 73 (2016)
and JQSRT **255**, 107228 (2020)

ExoMol database features

www.exomol.com

1. Line lists
2. Cross-sections
3. Partition functions
4. Broadening parameters
   (Barton et al, JQSRT **187**, 453 & 203, 490 (2017))
   H_2 and He: J and T dependence (only)
5. k-tables
6. Lifetimes (Tennyson et al, J Phys B, 49, 044002 (2016))
7. Cooling functions
8. Lande g-factors (Semenov et al, J Mol Spectrosc (2016))
9. Dipoles for molecular control/orientation effects
   A Yachmenev, RichMol project (Owens et al, Sci Rep 7, 45068 (2017))
10. Application program interface (API)
11. Opacity tables (in 4 formats) (Chubb et al. *A&A*, **646**, A21 (2021))
12. LiDa: Lifetimes database
13. ExoMolHR: high resolution spectra
14. New! Temperature dependent photodissociation cross sections

E-science Infrastructures

European Open Science Cloud

VESPA from EuroPlanet imbedding SSHADE : database for solid spectroscopy

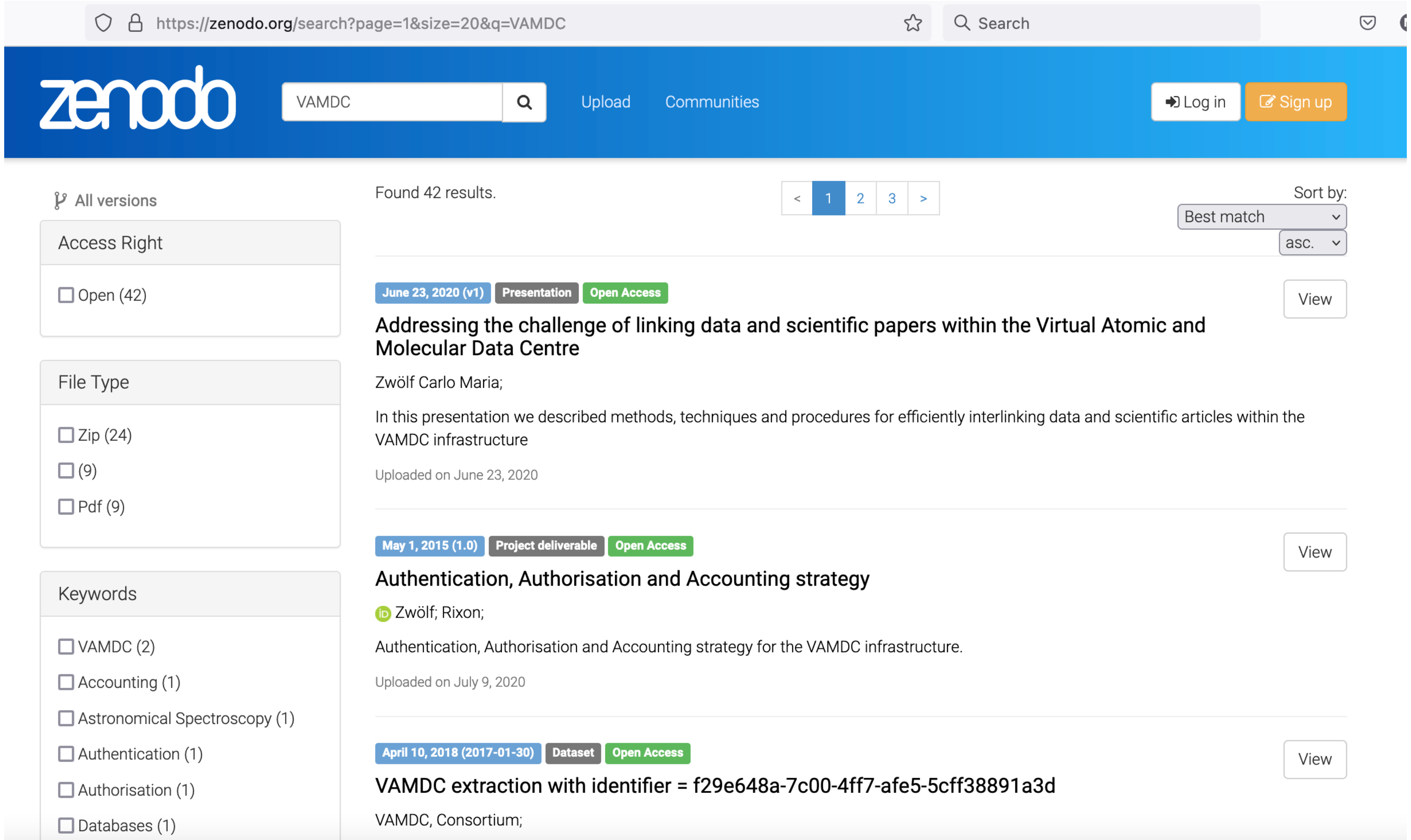
(http://vespa.obspm.fr/planetary/data/, https://www.sshade.eu/) –

VESPA : Provided by S. Erard and snapshot of SSHADE

VAMDC : an e-science platform for the exchange of Atomic and Molecular Data (vamdc.org)

ML Dubernet : Chair of VAMDC and VAMDC Collaboration (http://www.vamdc.org)

ZENODO



https://zenodo.org/search?page=1&size=20&q=VAMDC
Search
zenodo
VAMDC
Upload
Communities
Log in
Sign up
All versions
Access Right
Open (42)
File Type
Zip (24)
(9)
Pdf (9)
Keywords
VAMDC (2)
Accounting (1)
Astronomical Spectroscopy (1)
Authentication (1)
Authorisation (1)
Databases (1)
Found 42 results.
< 1 2 3 >
Sort by:
Best match
asc.
June 23, 2020 (v1)
Presentation
Open Access
View
Addressing the challenge of linking data and scientific papers within the Virtual Atomic and Molecular Data Centre
Zwölf Carlo Maria;
In this presentation we described methods, techniques and procedures for efficiently interlinking data and scientific articles within the VAMDC infrastructure
Uploaded on June 23, 2020
May 1, 2015 (1.0)
Project deliverable
Open Access
View
Authentication, Authorisation and Accounting strategy
Zwölf; Rixon;
Authentication, Authorisation and Accounting strategy for the VAMDC infrastructure.
Uploaded on July 9, 2020
April 10, 2018 (2017-01-30)
Dataset
Open Access
View
VAMDC extraction with identifier = f29e648a-7c00-4ff7-afe5-5cff38891a3d
VAMDC, Consortium;

EOSC Portal : https://eosc-portal.eu/

The European Open Science Cloud (EOSC) is an environment for hosting and processing research data to support EU science.

The ambition of the European Open Science Cloud (EOSC) is to provide European researchers, innovators, companies and citizens with a federated and open multi-disciplinary environment where they can publish, find and re-use data, tools and services for research, innovation and educational purposes.

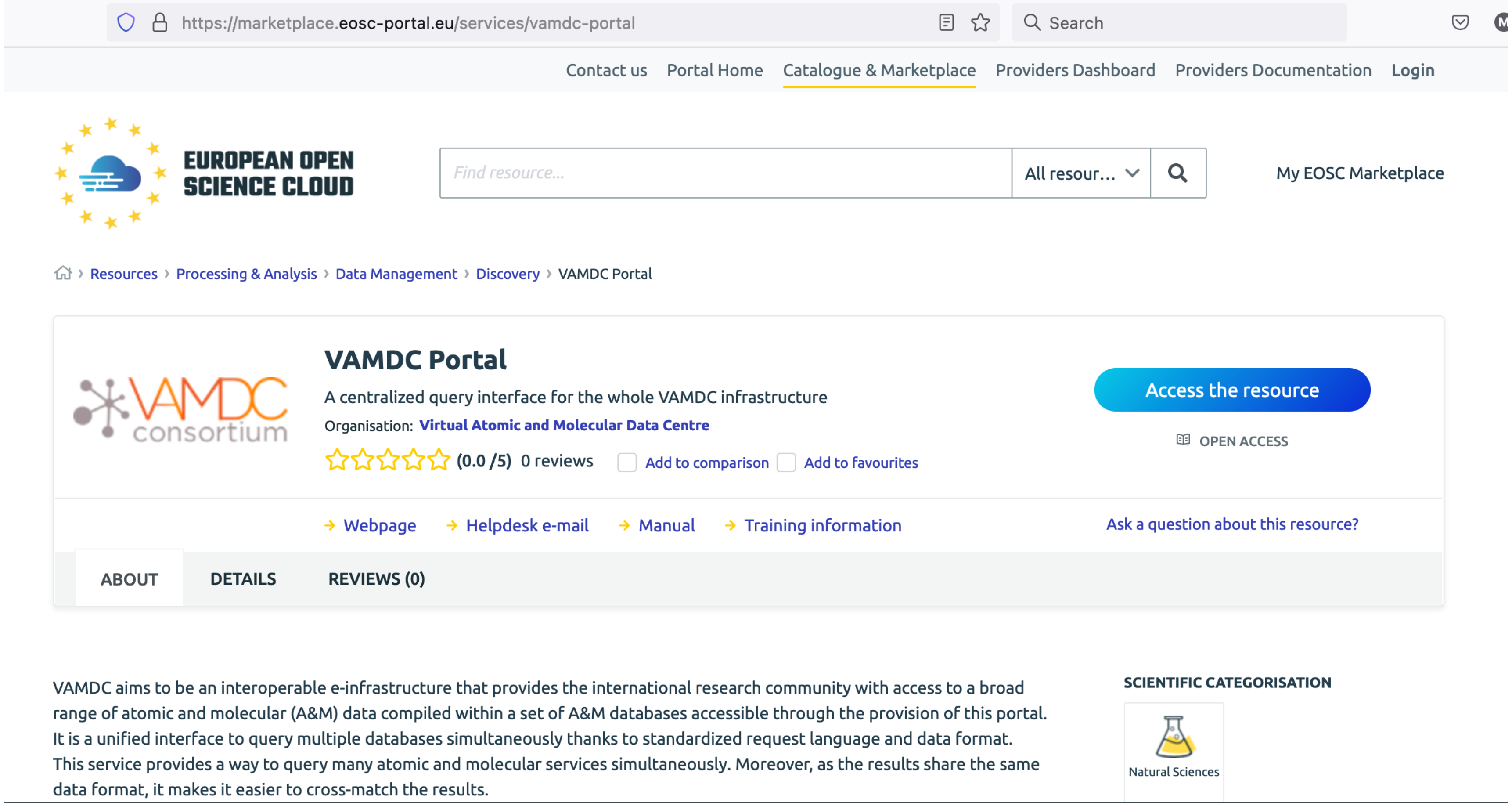
This environment will operate under well-defined conditions to ensure trust and safeguard the public interest.

The EOSC enables a step change across scientific communities and research infrastructures towards

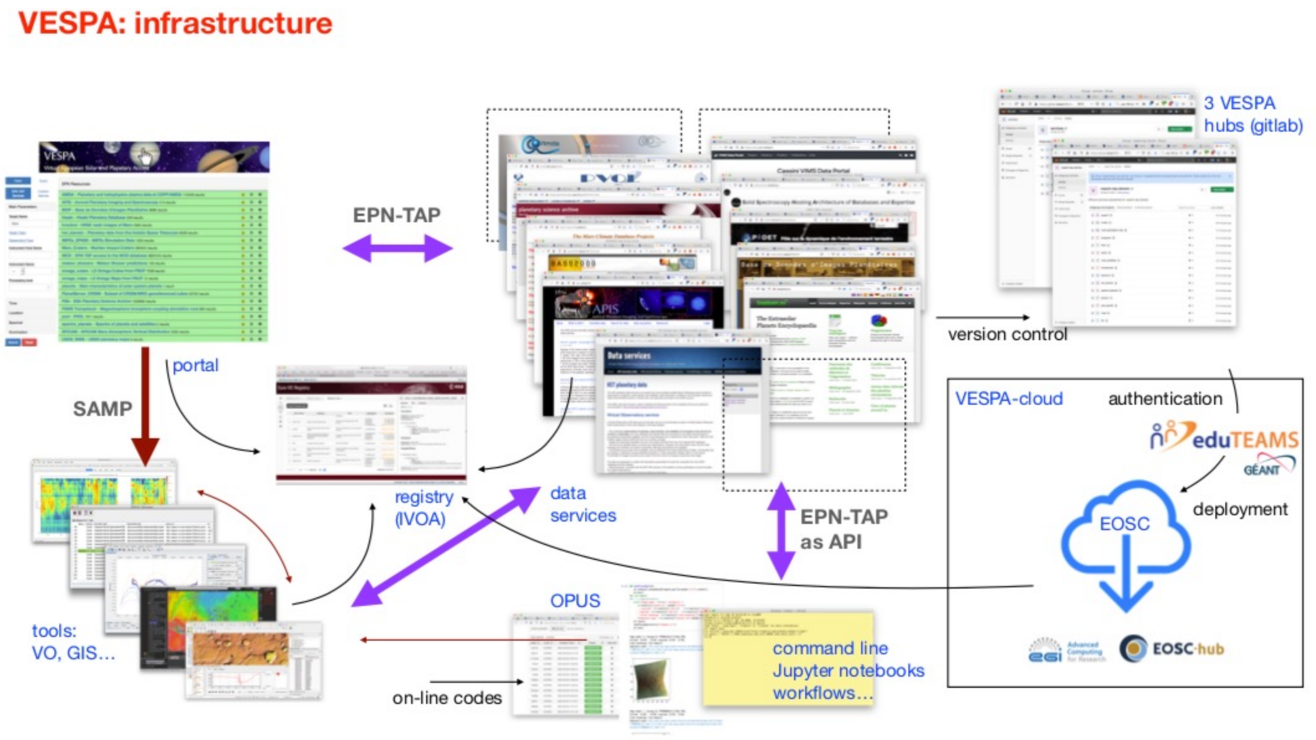
- seamless access
- FAIR (Findability, Accessibility, Interoperability and Reusability) management
- reliable reuse of research data and all other digital objects produced along the research life cycle (e.g. methods, software and publications)

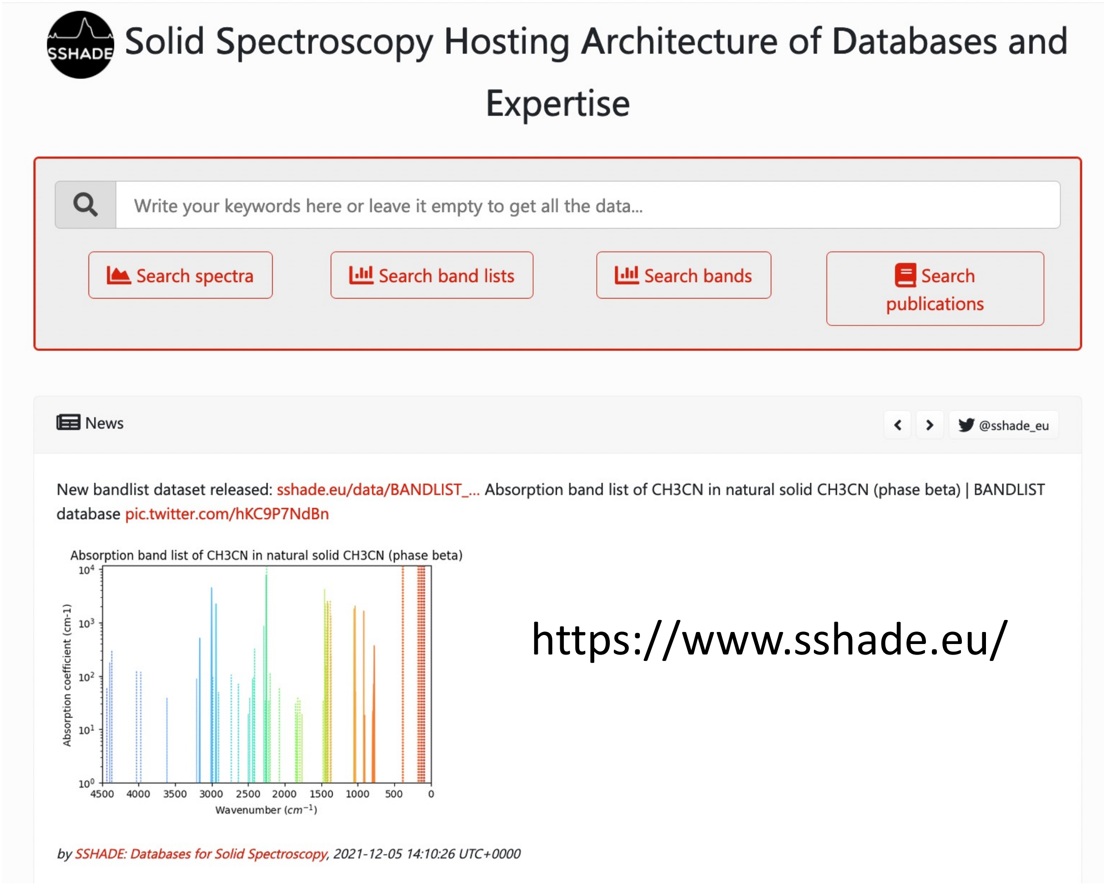
https://ec.europa.eu/info/research-and-innovation/strategy/strategy-2020-2024/our-digital-future/open-science/european-open-science-cloud-eosc_en

EOSC Market Place



VESPA from EuroPlanet : imbedding SSHADE





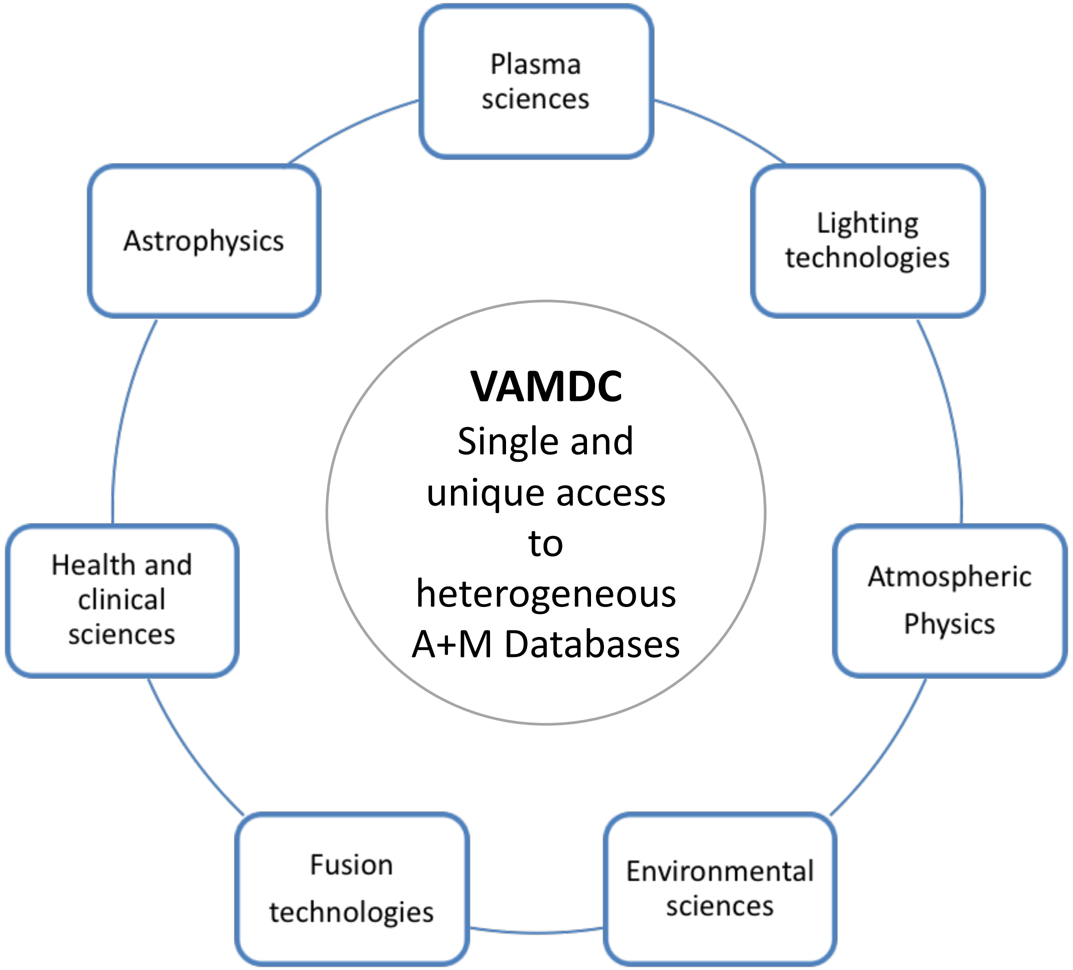
https://www.sshade.eu/

Virtual Atomic and Molecular Data Center - VAMDC

http://www.vamdc.org

Paper « A decade with VAMDC : results and ambition, Atoms, 2020 »
http://dx.doi.org/10.3390/atoms8040076.

The Virtual Atomic and Molecular Data Centre http://www.vamdc.org



- Federates ~37 heterogeneous databases http://portal.vamdc.org/
- The "V" of VAMDC stands for Virtual in the sense that the e-infrastructure does not contain data. The infrastructure is a wrapping for exposing in a unified interoperable way a set of heterogeneous databases.
- The consortium is politically organized around a Memorandum of understanding (15 international members have signed the MoU in 2014, 7 partners and 5 partners to come)
- High quality scientific data come from different Physical/Chemical Communities
- Provides data producers with a large dissemination platform

VAMDC consortium

VAMDC CONNECTED DATABASES

tabases	Type of A&M Data	Partners	Application's Fields
NIFS AMDIS IONIZATION	Electron-impact ionization cross-sections and rate coefficients (atoms & atomic ions)	National Institute for Fusion Science, Toki, Japan, I. Murakami	Stellar, Solar, plasma, fusion
VALD	Atomic Linelists	Uppsalla, Vienna, Moscow – N. Piskunov	Stellar –Solar
NIST Atomic Spectra	Spectroscopy of Atoms –	NIST – Yuri Ralchenko	Stellar – ISM -
CHIANTI	Atomic Linelists and collisions	Cambridge (UK)+MSSL/UCL – H. Mason, G. Rixon	Solar Physics
Spectr-W3	Atomic Linelists and Collisions	Russia (RFNC VNIITF) – P. Loboda	Solar/Stellar Physics + Fusion, plasma
Stark-B	Atomic LineShifts/Broadening with charged perturbers	Observatory of Belgrade (Serbia) + Observatory of Paris (LERMA) – M. Dimitrijevic/S. Sahal-Bréchot	Stellar Physics + Plasmas
TipBase, TopBase	Atomic Linelists and Collisions from Opacity Project and IRON Project	Observatory of Paris (LERMA) + CDS (Strasbourg, Fce) – F. Delahaye/C. Zeippen/C. Mendoza	Stellar, Solar Physics,
SESAM	Electronic Spectra of atoms and molecules	Paris Obs. – E. Roueff	ISM - Stellar

VAMDC consortium

VAMDC CONNECTED DATABASES

Databases	Type of A&M Data	Partners	Application's Fields
MOLD	Photo-Dissociation Cross-sections	Institute of Physics, Astronomical Obs, Belgrade, Serbia- Vladimir Sreckovic, V. Vujcic, D. Jevremovic	Stellar
BEAM-DB	Molecular/atom—electron collisions	Institute of Physics, Belgrade, Serbia Bratislav Marinkovi\'c	plasma, radiation damage
IDEABD	Dissociative electron attachment upon interaction of low energy electrons with molecules.	Innsbrück F. Duensing	Planets, ExoPlanets, ISM, Radiation Damage

VAMDC CONNECTED DATABASES

Databases	Type of A&M Data	Partners	Application's Fields
CDMS	Molecular Linelists (mm, Sub-mm)	Cologne (Germany) – S. Schlemmer	ISM + Earth+ CO
JPL	Molecular Linelists (mm, Sub-mm)	Pasadena (USA) + Cologne (Germany) – B. Drouin	ISM + Earth+CO
HITRAN	Molecular Linelists and Broadening Coefficients	Harvard (USA) + UCL – I. Gordon + L. Rothman	Earth, Planets, Exo-Planets
S&MPO	O_3 linelists	Reims (France)+ Tomsk (Russia) – V. Tyuterev	Earth – Exo-Planets
MeCaSDa	Linelists CH_4	Dijon (France) – V. Boudon	Earth, Planets, Exo-Planets, Brown dwarfs
SHeCaSDa	Sulfur Hexafluoride Calculated LInelists	Dijon – V. Boudon	Earth
TFMeCaSDa	Tetrafluoro-Methane calculated linelists	Dijon – V. Boudon	Earth
ECaSDa	Ethene Calculated LInelists	Reims – L. Daumont	Earth and Planets
GeCaSDa	GeH_4 Linelists	Dijon – V. Boudon	Planets

VAMDC CONNECTED DATABASES

Databases	Type of A&M Data	Partners	Application's Fields
RuCaSDa	RuO_4 Linelists	Dijon – V. Boudon	Nuclear Industry
TFSiCaSDa	SiF_4 Linelists	Dijon – V. Boudon	Earth
UHeCaSDa	UF_6 Linelists	Dijon – V. Boudon	Nuclear Industry
CDSD-296	CO_2 Linelists (intensity cut-off)	IAO, Tomsk – V. Perevalov	Earth, Planets, Brown Dwarfs
CDSD-1000	CO_2 Linelists (intensity cut-off)	IAO, Tomsk – V. Perevalov	Earth, Planets, Brown Dwarfs
CDSD-4000	CO_2 Linelists (intensity cut-off)	IAO, Tomsk – V. Perevalov	Earth, Planets, Brown Dwarfs
NOSD-1000	N_2O Linelists (intensity cut-off)	IAO, Tomsk – V. Perevalov	Earth, Planets
NDSD-1000	NO_2 Linelists (intensity cut-off)	IAO, Tomsk – V. Perevalov	Earth, Planets
ASD-1000	C_2H_2 Linelists (intensity cut-off)	IAO, Tomsk – V. Perevalov	Earth, Planets

VAMDC CONNECTED DATABASES

Databases	Type of A&M Data	Partners	Application's Fields
PAH	PAH Theoretical Data and soon experimental Data	Observatory of Cagliari (Italy) – IRAP (Toulouse, France) – G. Mulas+C. Joblin	ISM, Planets, Earth
KIDA	Kinetic Data	Bordeaux (France) – P. Gratier & V. Wakelam	ISM - Planets
UdfA	Kinetic Data (ex-UMIST)	Belfast (UK) – T. Millar	ISM - Planets
BASECOL	Low Energy Molecular Collisions	Observatory of Paris – M.L. Dubernet	ISM - CO
LASP	Solid Spectroscopy Data	Obs. of Catania – G. Leto	Planets, ISM
GhoSST	Solid Spectroscopy Data	Grenoble (France) – B. Schmitt	Planets, ISM
W@DIS	Water Information System	IAO, Tomsk – A. Fazliev	Earth and Planets

To be connected to VAMDC e-infrastructure

Databases	Type of A&M Data	Partners	Application's Fields
ExoMolOP	Molecular Opacities	University College London, UK – J. Tennyson	Exo, Brown Dwarf, Earth, Stellar
SSHADE	Solid Spectroscopy Data - Interface to infrastructure	Grenoble (France) & other countries – B. Schmitt et al	Earth, Comets, Exo-Planets, ISM, Planets
IAMDB	Indian Atomic and Molecular Database (atomic collisions, A+M spectroscopy)	B. Antony- Indian Institute of Technology, Dhanbad, India E. Krishnakumar - Raman Research Institute, Bengalore, India	Astrophysics, Other
AMBDAS	Collisions in plasmas (bibliographic) - searchable via processes ans species	IAEA, Vienna, Austria - C. Hill	Nuclear Fusion
DESIRE	Spectroscopy of sixth row elements (Z=72-86)	Mons University and Liege University, Belgium – P.Quinet, P. Palmeri	Plasmas – Stellar - Solar
DREAM	Radiative data for rare earth	Mons University and Liege University, Belgium – P Quinet, P. Palmeri	Stellar-Solar-Plasmas – Lighting -

To be connected to VAMDC e-infrastructure

Databases	Type of A&M Data	Partners	Application's Fields
PEARL	Atomic Processes	Nuclear data Center, KAERI, Daejon, South Korea Kwon Duck-Hee	Stellar-Solar-Plasmas – Fusion
Clusters	Cluster size distributions, condensation	Innsbrück F. Duensing, P. Scheier	Planets, ExoPlanets, Solvation, Biology
Additional NIFS Databases	Atomic/Molecular processes	National Institute for Fusion Science, Toki, Japan, I. Murakami	Stellar, Solar, plasma, fusion

VAMDC and the FAIR principle

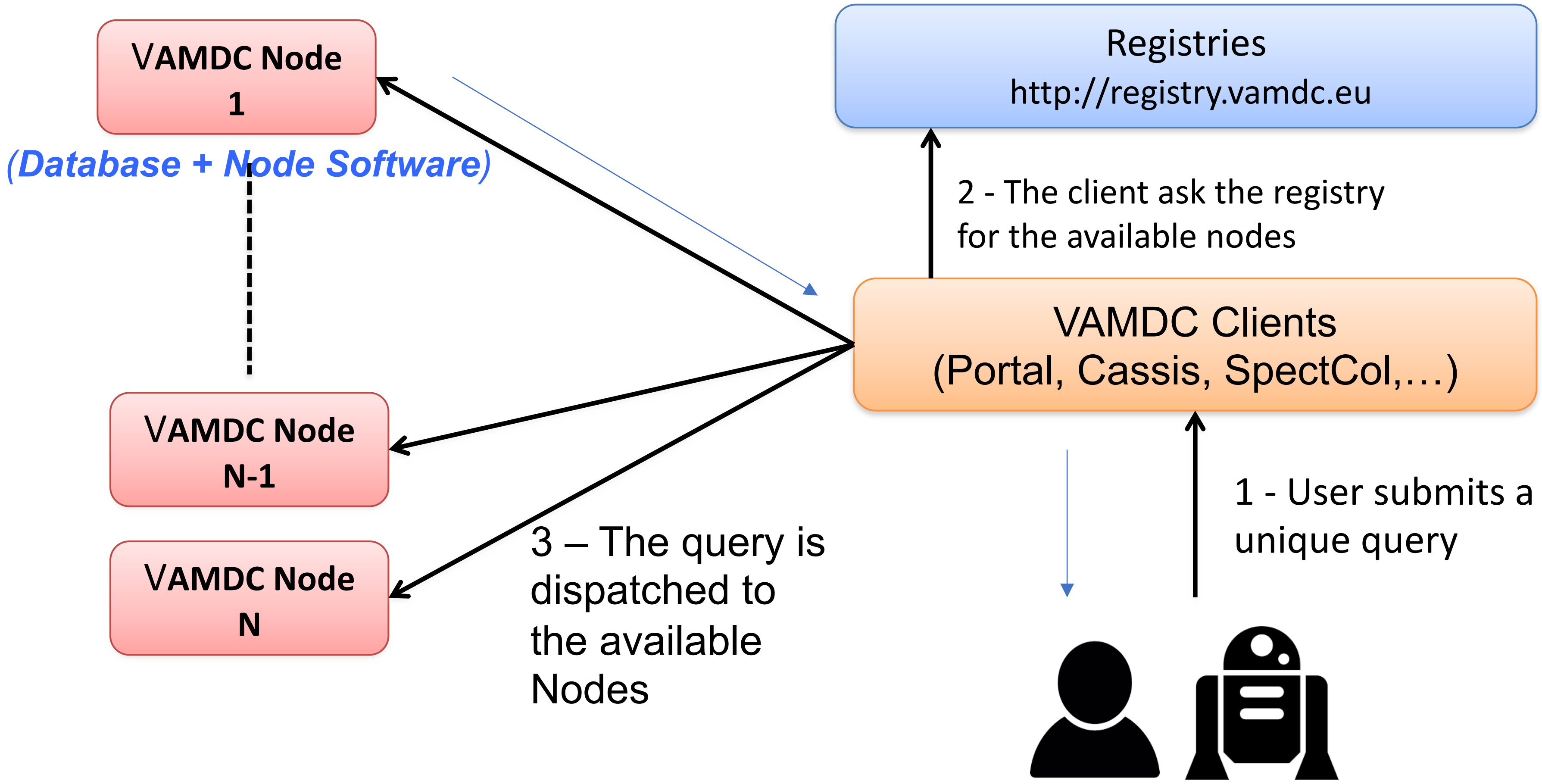
FAIR (Findability, Accessibility, Interoperability, Reuse) principles underlined the design of VAMDC

- Findable : data coming from the infrastructure can be tagged with persistent unique identifiers, are described with rich metadata and are indexed into public registries
- Accessible : the extraction query relies on open, documented standards
- Interoperable : the data extracted from VAMDC are formatted using the XSAMS standard
- Re-usable : the provenance and sources of all the data are documented in each data set extracted from VAMDC. Data tools are provided to convert VAMDC data into widely adopted community data formats

VAMDC Technical Infractructure

- A set of standards
  - Data exchange Protocols, Data Description
  - Standard vocabulary for all exchanges, including for registration of ressources
- A set of software (www.vamdc.org/software)
- Documentation and on-line support system (www.vamdc.eu)
- Monitoring of services and support (support@vamdc.eu)

The VAMDC infrastructure technical architecture relies on Standards



Courtesy of C.M. Zwolf

STANDARDS

www.vamdc.org/standards

Home | About Us | Services | News | Contact

You are here > Services > Research > Documents > **Standards**

RESEARCH SERVICES

Access to Data
- VAMDC Research Portal
- RADAM Portal

Software
- SPECTCOL
- SPECVIEW
- XSAMS Converter
- PDL-VAMDC
- JavaScriptPortal
- TAPValidator
- Java NodeSoftware
- Python NodeSoftware
- Libraries
- Virtual machines for node building

Documents
- Standards
- Science use cases
- Tutorials
- See our videos
- FAQ

STANDARDS

VAMDC standards are a set of norms, protocols, regulations which are the basis of the VAMDC-infrastructure operations.

Follow the links below for further information on each item of the following list:

- VAMDC standards documentation page
  - VAMDC documentation and software versioning policy
  - Data access protocol, query language and dictionaries
  - Data model
  - Registry
  - Units
  - InChI Generation
  - XSAMS Processor service

Official citation of VAMDC standards

The official citation of VAMDC standards is:

"M. L. Dubernet, M. Doronin, C. Endres, C. Hill, T. Marquart, L. Nenadovic, Y. Ralchenko, G. Rixon and K. Smith, VAMDC Standards Documentation and Reference Guides, version r12.07, Virtual Atomic and Molecular Data Centre, http://standards.vamdc.eu (2012)"

ACCESS TO THE PORTAL

Access to VAMDC databases

Portal Access

ACCESS TO THE SPECIES DATABASE

List of species in each VAMDC database

Species Access

VAMDC consortium

Data Description : XSAMS format

XML Schema for Atoms Molecules and Solids

XSAMS is a rigorous and unambiguous object model for atomic and molecular physics

- Any VAMDC output is a valid XSAMS file.
- This Standardisation is a joint effort involving initially NIST, IAEA, ORNL, Observatoire de Paris, VNIITF and then VAMDC

VAMDC consortium

20/25 Groups

IAEA
International Atomic Energy Agency

R.E.H. Clark,
D. Humbert
B. Braams

NIST National Institute of Standards and Technology U.S. Department of Commerce

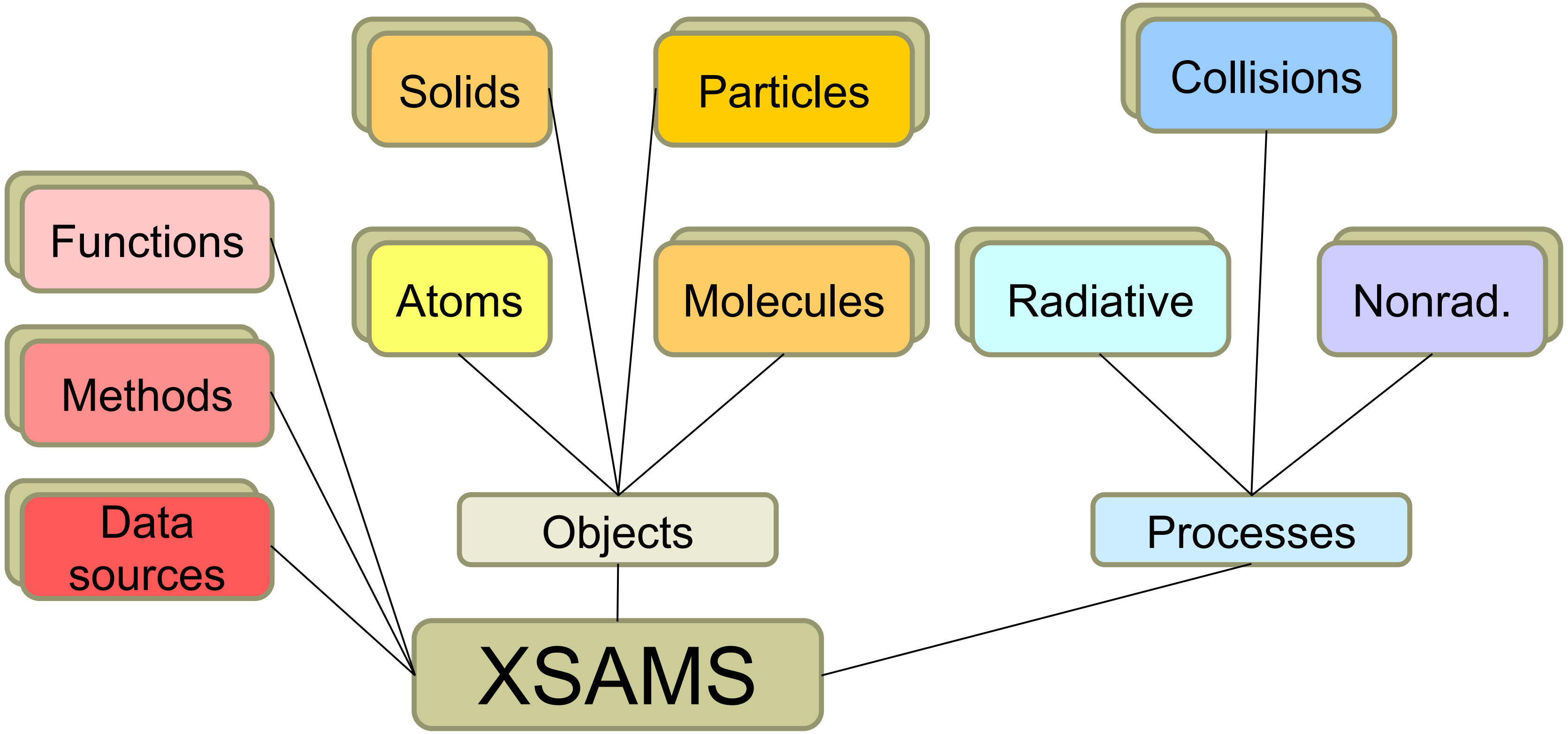
Y. Ralchenko

D.R. Schultz, ORNL

E. Roueff, ML Dubernet, Observatoire Paris

S. Gagarin, P.A. Loboda, VNIITF

XSAMS tree: XML Schema for Atoms, Molecules and Solids



(Courtesy Yuri Ralchenko)

Dictionnaries associated to Queries

Restrictables

The following keywords may be used as **restrictables** in TAP-VAMDC queries using VSS1 language, also they are added to registry for each new node.

Note that each node supports only a small subset of the keywords. The list of supported keywords may be retrieved through **VOSI Capabilities** service endpoint. See the TAP-VAMDC documentation for further details.

AsOfDate

Return data excluding any additions or improvements that were made after the given date (YYYY-MM-DD). This allows for reproducing an earlier query. Note that probably not all nodes support this.

Type: string

Constraints:

AtomMass

The atomic mass is the mass of an atom expressed in unified atomic mass unit u. It is defined as 1/12 of the rest mass of an unbound carbon-12 atom in its nuclear and electronic ground state. 1 u = 1.660538782(83)E-27 kg.

Units: u

Type: floating-point number

Constraints: >1

AtomMassNumber

Atomic mass number (A), also called mass number or nucleon number, is the total number of protons and neutrons (together known as nucleons) in an atomic nucleus. Because protons and neutrons both are baryons, the mass number A is identical with the baryon number B as of the nucleus as of the whole atom or ion. The mass number is different for each different isotope of a chemical element.

Type: integer number

Table Of Contents

VAMDC Tools

Portal

SPECTCOL Tool

Species Database

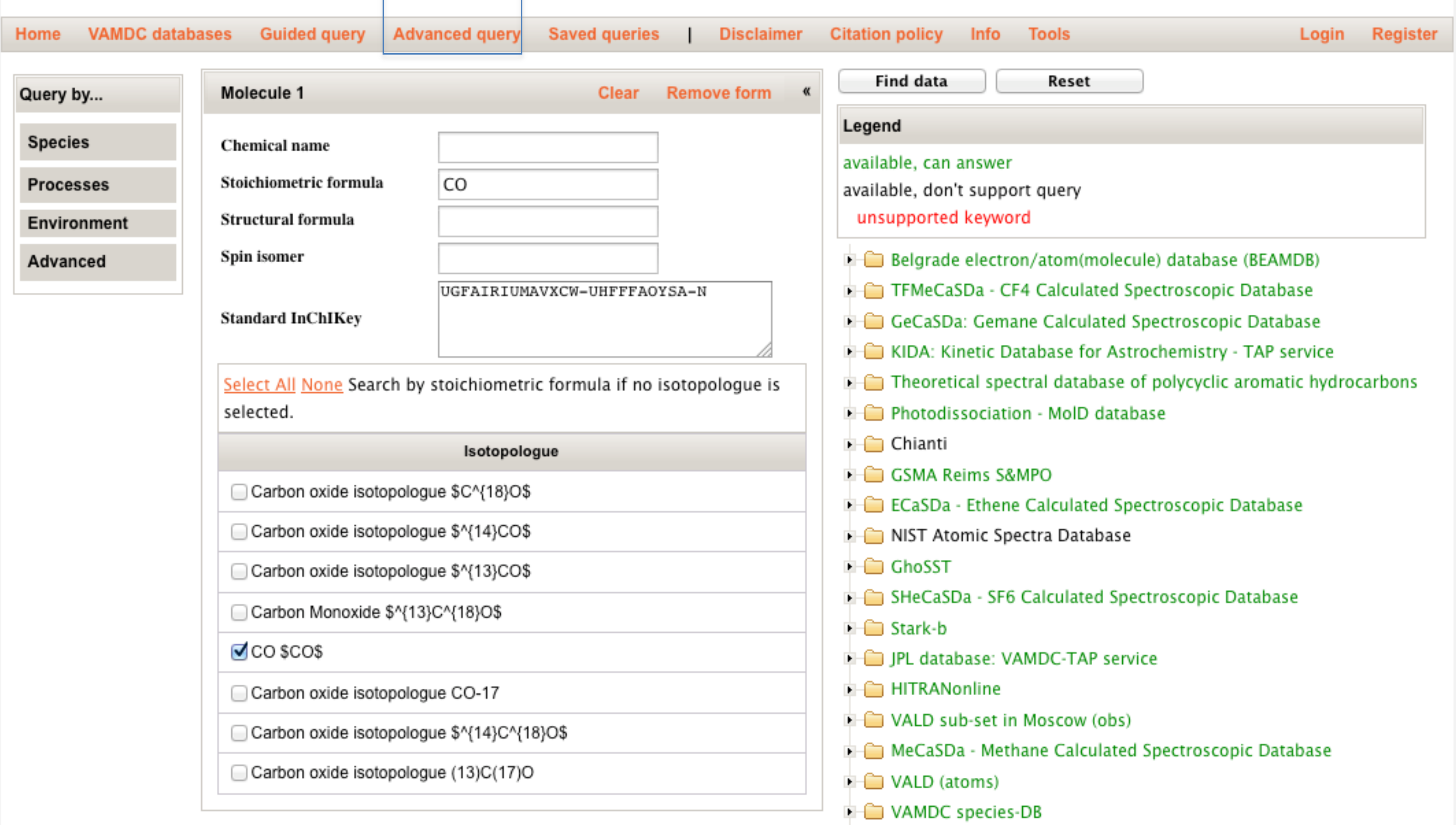
Query Store

Bibliographic Service (in development)

Current Search & Display Version

Capabilities linked to the amount of effort of the different VAMDC communities

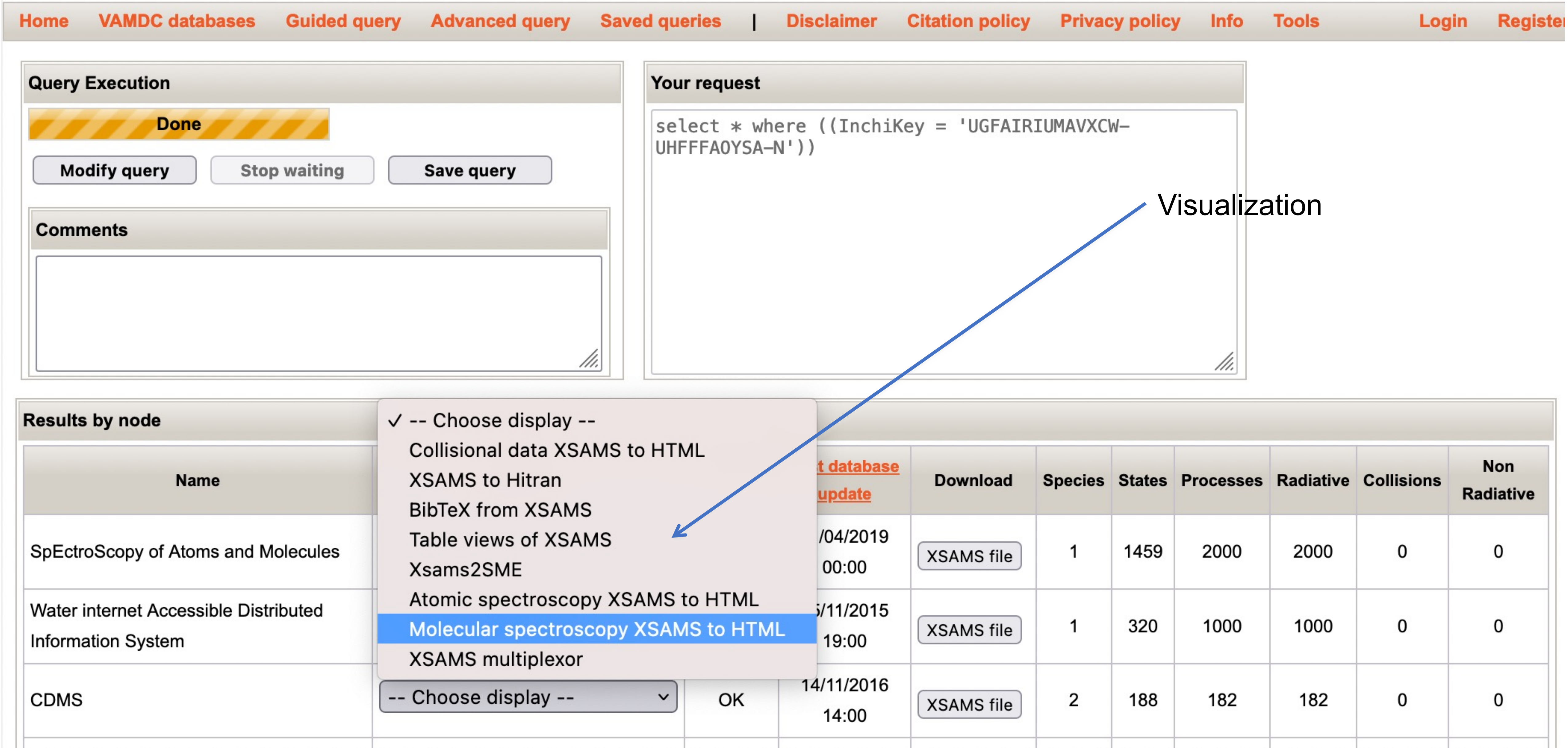
Portal : portal.vamdc.eu



Currently maintained : N. Moreau

VAMDC consortium

TABLE of Databases answering the « CO » request



Menu

- Export as CSV
- Export as JSON
- Export as VOTable
- Send with samp
- Reset page

Different formats to export data

Including IVOA VOTable

Sources

Id	Title	Origin	Authors	Year	Link
BCDMS-178	Infrared CO line for the X 1 Sigma(+) state	journal : Astrophys. J. Suppl. (Vol : 95 , Page Begin : 535)	Goorvitch, D.;	1994	http://xsams-processors.obspm.fr/applyXSL/molecularxsams2html/result/3232?ivoaID=ivo%3A%2F%2Fvamdc%2Fcdms%2Fvamdc-tap_12.07
BCDMS-921	Accurate laboratory rest frequencies of vibrationally excited CO up to v= 3 and up to 2 THz	journal : Astron. Astrophys. (Vol : 497 , Page Begin : 927 , Page End : 930)	Gendriesch, R.; Lewen, F.; Klapper, G.; Menten, K. M.; Winnewisser, G.; Coxon, J. A.; Müller, H. S. P.;	2009	http://xsams-processors.obspm.fr/applyXSL/molecularxsams2html/result/3232?ivoaID=ivo%3A%2F%2Fvamdc%2Fcdms%2Fvamdc-tap_12.07
BCDMS-1681	Sub-Doppler Measurements on the Rotational Transitions of Carbon Monoxide?	journal : J. Mol. Spectrosc. (Vol : 184 , Page Begin : 468)	Winnewisser, G.; Belov, S. P.; Klaus, T.; Schieder, R.;	1997	http://xsams-processors.obspm.fr/applyXSL/molecularxsams2html/result/3232?ivoaID=ivo%3A%2F%2Fvamdc%2Fcdms%2Fvamdc-tap_12.07
BCDMS-1919	The rQ4Branch of HSSH at 1.25 THz	journal : J. Mol. Spectrosc. (Vol : 174 , Page Begin : 606 , Page End : 612)	Belov, S.P.; Lewen, F.; Klaus, T.; Winnewisser, G.;	1995	http://xsams-processors.obspm.fr/applyXSL/molecularxsams2html/result/3232?ivoaID=ivo%3A%2F%2Fvamdc%2Fcdms%2Fvamdc-tap_12.07
BCDMS-1920		private communication : 52nd Okaz Okaz	Evenson, K. M.;	1995	http://xsams-processors.obspm.fr/applyXSL
BCDMS-1921	CDMS database	da			
BCDMS-2709	The Cologne Database for Molecular Spectroscopy, CDMS, in the Virtual Atomic and Molecular Data Centre, VAMDC	journal : J. (Vol : 327 95 , Pag			

Results from CDMS VAMDC node

Unselect all	Chemical name X	Stoichiometric formula X	Or stru for

Using the

Molecular spectroscopy XSAMS to HTML

visualisation

Results from CDMS VAMDC node

Unselect all	Chemical name X	Stoichiometric formula X	Ordinary structural formula X	Frequency X	Frequency reference X	A X	Lower energy(1/cm) X	Lower total statistical weight X	Lower nuclear statistical weight X	Lower QNs X	Upper energy(1/cm) X	Upper total statistical weight X	Upper nuclear statistical weight X	Upper QNs X
☑	Carbon Monoxide	CO	CO	112123.0871		6.602636007873798e-09	6350.4391	1	1	ElecStateLabel=X v=3 J=0	6354.1791	3	1	ElecStateLabel=X v=3 J=1
☑	Carbon Monoxide	CO	CO	113172.3761		2.0046120206563544e-08	4260.0622	1	1	ElecStateLabel=X v=2 J=0	4263.8372	3	1	ElecStateLabel=X v=2 J=1
☑	Carbon Monoxide	CO	CO	114221.7523		4.179185708685541e-08	2143.2711	1	1	ElecStateLabel=X v=1 J=0	2147.0811	3	1	ElecStateLabel=X v=1 J=1
☑	Carbon Monoxide	CO	CO	115271.2018	BCDMS-1681	7.20360334988053e-08	0.0	1	1	ElecStateLabel=X v=0 J=0	3.845033	3	1	ElecStateLabel=X v=0 J=1
☑	Carbon Monoxide	CO	CO	224241.7699		6.326402296865408e-08	6354.1791	3	1	ElecStateLabel=X v=3 J=1	6361.659	5	1	ElecStateLabel=X v=3 J=2
☑	Carbon Monoxide	CO	CO	226340.341		1.921670231723644e-07	4263.8372	3	1	ElecStateLabel=X v=2 J=1	4271.3871	5	1	ElecStateLabel=X v=2 J=2
☑	Carbon Monoxide	CO	CO	228439.074		4.0091218869191427e-07	2147.0811	3	1	ElecStateLabel=X v=1 J=1	2154.701	5	1	ElecStateLabel=X v=1 J=2
☑	Carbon Monoxide	CO	CO	230538	BCDMS-1681	6.910612264742753e-07	3.845033	3	1	ElecStateLabel=X v=0 J=1	11.534953	5	1	ElecStateLabel=X v=0 J=2
☑	Carbon Monoxide	CO	CO	336351.6444		2.2795543037921695e-07	6361.659	5	1	ElecStateLabel=X v=3 J=2	6372.8785	7	1	ElecStateLabel=X v=3 J=3
☑	Carbon Monoxide	CO	CO	339499.521		6.935117970601795e-07	4271.3871	5	1	ElecStateLabel=X v=2 J=2	4282.7116	7	1	ElecStateLabel=X v=2 J=3
☑	Carbon Monoxide	CO	CO	342647.636		1.4474584063103772e-06	2154.701	5	1	ElecStateLabel=X v=1 J=2	2166.1305	7	1	ElecStateLabel=X v=1 J=3
☑	Carbon Monoxide	CO	CO	345795.9899	BCDMS-1681	2.4966366421259645e-06	11.534953	5	1	ElecStateLabel=X v=0 J=2	23.069466	7	1	ElecStateLabel=X v=0 J=3
☑	Carbon Monoxide	CO	CO	448448.307		5.576286275994585e-07	6372.8785	7	1	ElecStateLabel=X v=3 J=3	6387.8371	9	1	ElecStateLabel=X v=3 J=4
☑	Carbon Monoxide	CO	CO	452645.4717		1.7002137582246867e-06	4282.7116	7	1	ElecStateLabel=X v=2 J=3	4297.8102	9	1	ElecStateLabel=X v=2 J=4
☑	Carbon Monoxide	CO	CO	456842.977		3.550670195309452e-06	2166.1305	7	1	ElecStateLabel=X v=1 J=3	2181.3692	9	1	ElecStateLabel=X v=1 J=4

SPECTCOL TOOL (new release 2022)

- Non-LTE Analysis of Astrophysical Spectra requires **Combined spectroscopic and collision Data**
- The Tool takes data through VAMDC from CDMS, JPL, HITRAN for spectroscopy and from BASECOL for collision
- The Tool **compares the energy levels via the quantum numbers**, so it is able to identically label the spectroscopic and the collisional transitions
- The tool creates output files in a customized format → Including IVOA VOtable
- Contact :
- Y.A. Ba yaye-awa.ba@obspm.fr
- ML Dubernet (Obs Paris)

VAMDC consortium

Species Database
https://species.vamdc.eu

Home Nodes Species Credits Data policy Help

Search

All nodes

Species

He

Mass min

Mass max

Charge min

1

Charge max

1

Submit

AMDIS Ionization (Atomic states, Atoms, Collisions)

Name	Stoichiometric formula	Formula	InChI	Mass number	InChIKey	Charge
Helium positive ion 1	He	None	InChI=1S/He/q+1	4	QLNXTEZOQCZJBA -UHFFFAOYSA-N	1

Chianti (Atomic states, Atoms, Radiative transitions)

Name	Stoichiometric formula	Formula	InChI	Mass number	InChIKey	Charge
Helium positive ion 1	He	None	InChI=1S/He/q+1	4	QLNXTEZOQCZJBA -UHFFFAOYSA-N	1

TIPbase : VAMDC-TAP interface (Atomic states, Atoms, Collisions)

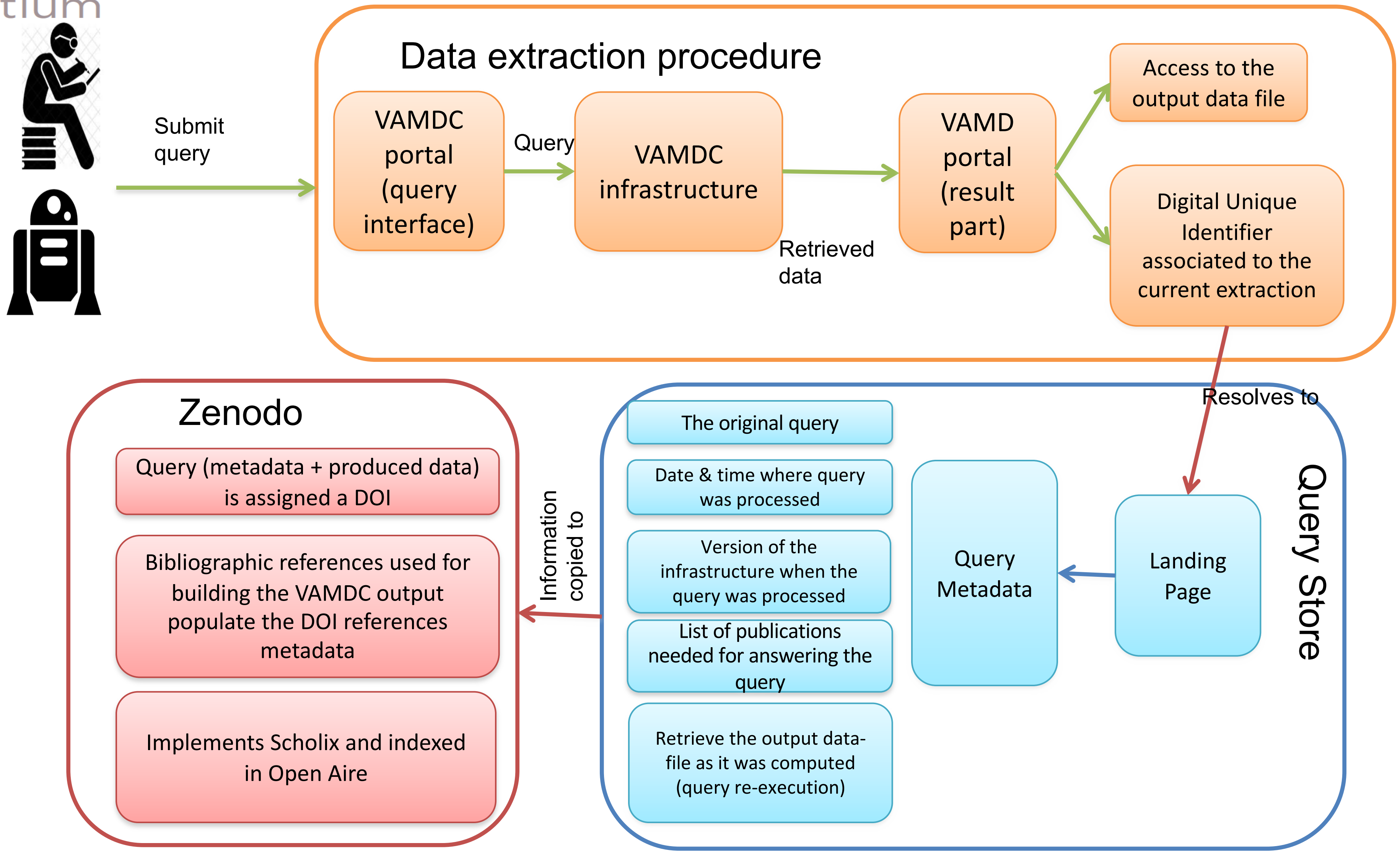
Name	Stoichiometric formula	Formula	InChI	Mass number	InChIKey	Charge
Helium positive ion 1	He	None	InChI=1S/He/q+1	4	QLNXTEZOQCZJBA -UHFFFAOYSA-N	1

TOPbase : VAMDC-TAP interface (Atomic states, Atoms, Cross sections, Radiative transitions)

Name	Stoichiometric formula	Formula	InChI	Mass number	InChIKey	Charge
Helium positive ion 1	He	None	InChI=1S/He/q+1	4	QLNXTEZOQCZJBA -UHFFFAOYSA-N	1

Currently maintained
N. Moreau

The VAMDC Query Store



- Data become directly citable by their DOI. Authors/papers referenced in the data-set will get credits automatically when the dataset is cited (using the DOI) into a paper

Courtesy of C.M. Zwolf

VAMDC 2022 On-going Activities

Very central activity and of utmost importance :
Maintenance of the VAMDC core services (Nicolas Moreau)

- Redundancy of VAMDC core services at Paris Observatory and at other places in the EU (N. Moreau, CM. Zwölf and VAMDC consortium)
- SPECTCOL Tool (Yaye Awa Ba, MLD)
- Inclusion of new DB : Japan&Korea (N. Moreau, MLD)
- Work on CoreTrustseal certification of VAMDC connected DB (Stark-B, BASECOL)
- Support to users (N. Moreau, MLD)
- "Mode asynchrone et SQL pour les gros volumes dans les services VAMDC-TAP"→ see hack-a-Thon (N. Moreau and VAMDC)
- "Mimic the VAMDC portal in a Google Colab notebook", Carlo Maria Zwölf → see hack-a-Thon
- New – This year – After 14 years since the start of VAMDC, leadership of VAMDC Consortium will go to Germany & IAEA

Information

- Report Bugs when you find them
  - support@vamdc.eu
- Do not hesitate to ask for help
  - To include new databases
  - For implementation of queries in your tools

- Infrastructure Technical Support and Standards
  - Paris Team : N. Moreau, Y. A. Ba, C. M. Zwölf
  - Cambridge Team : G. Rixon
  - Uppsala Team : T. Marquart
  - Cologne/Garching Team : C. Endres
  - IAEA : Case-by-Case : C. Hill
  - Dijon Team : C. Richard

Individual Databases : see nodes and contacts at https://portal.vamdc.eu/vamdc_portal/nodes.seam

For now any questions can be addressed to : support@vamdc.eu

XCLASS (Cologne, Provided by P. Schilke)

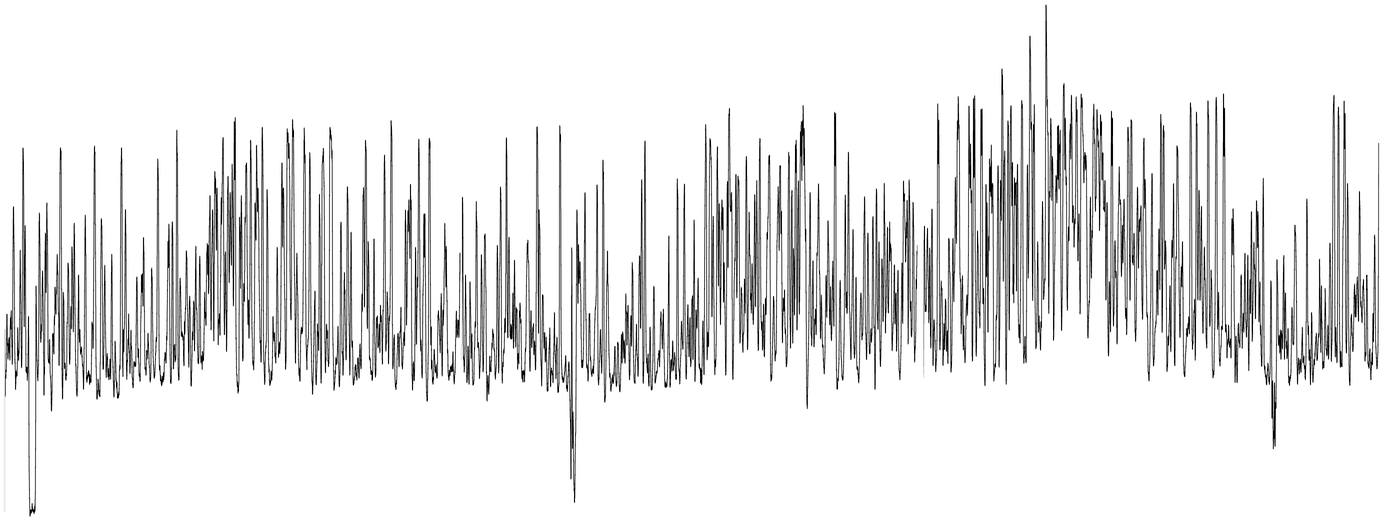
IRAM Suite and YaFITS (Grenoble & Obs Paris, provided by J. Pety and P. Salomé)

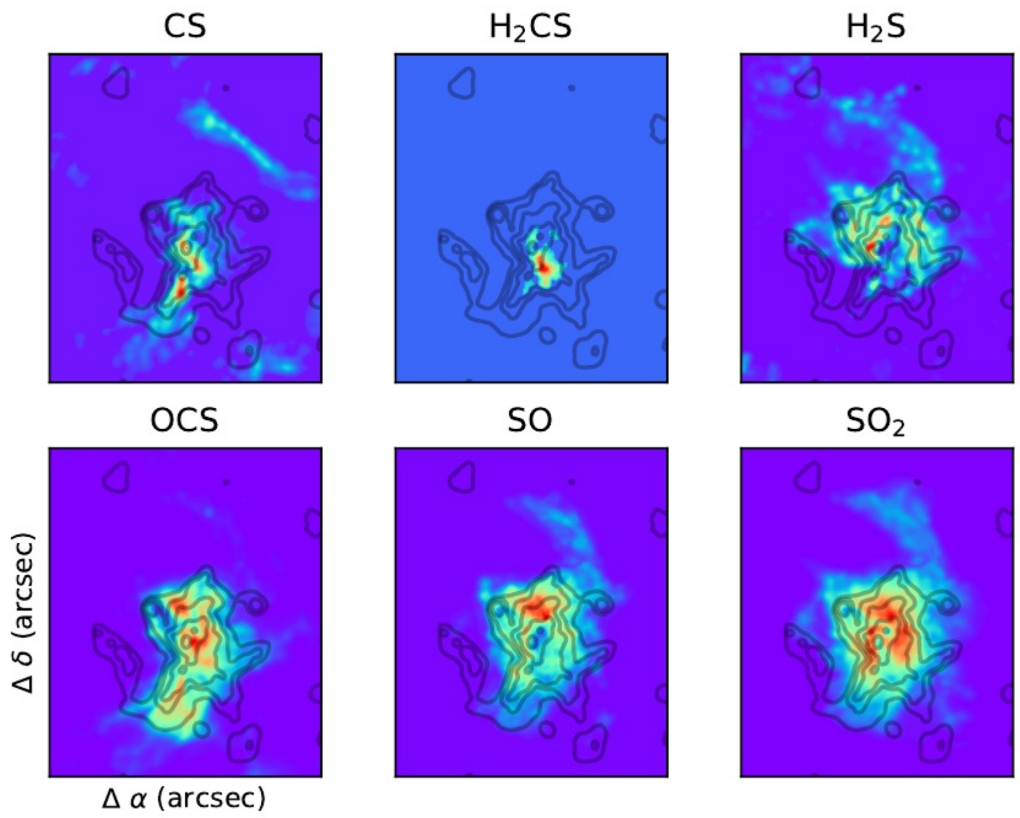
CASSIS (Toulouse, re-organised information from materials from J.M. Glorian)

ASTROPHYSICS SOFTWARE TOOLS (A&M EMBEDDED) –

Provided by P. Schilke

Challenge: analysis of complex spectra and maps





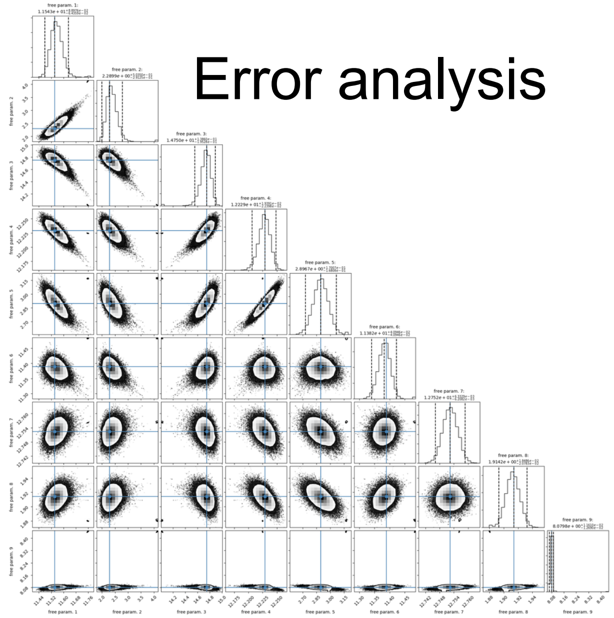
- Based on up-to-date molecular data
- Automatized
- Fast
- Reliable
- With quality control
- Reproducible

Solution: XCLASS

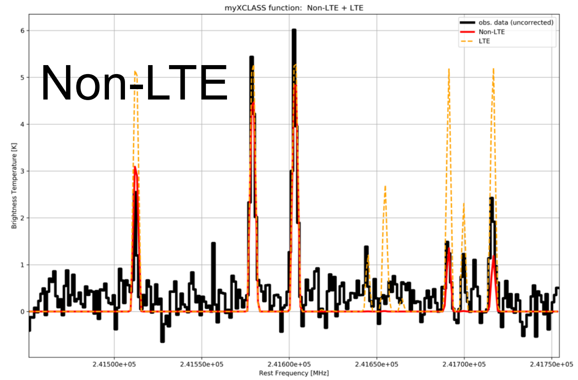
(P. Schilke and coll)

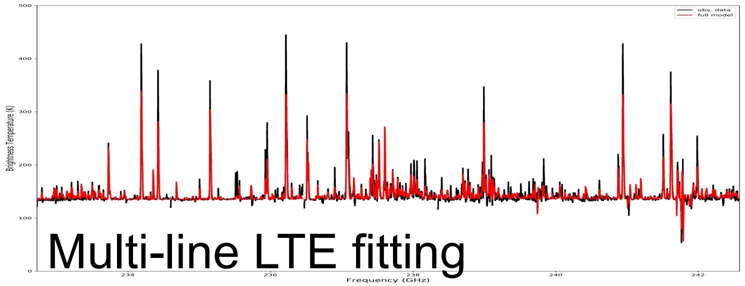
GUI

Error analysis

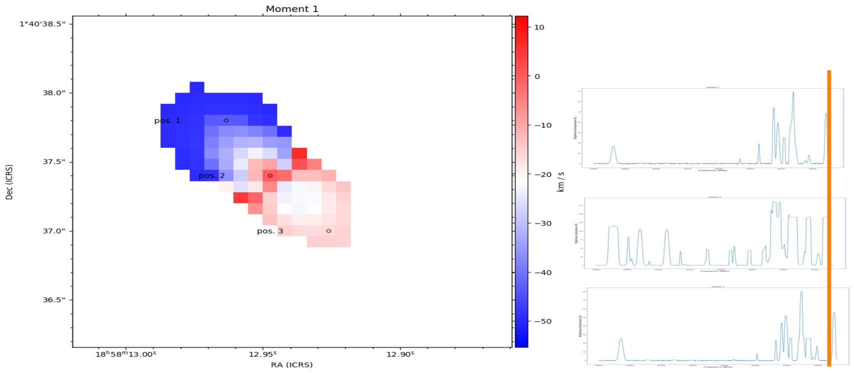


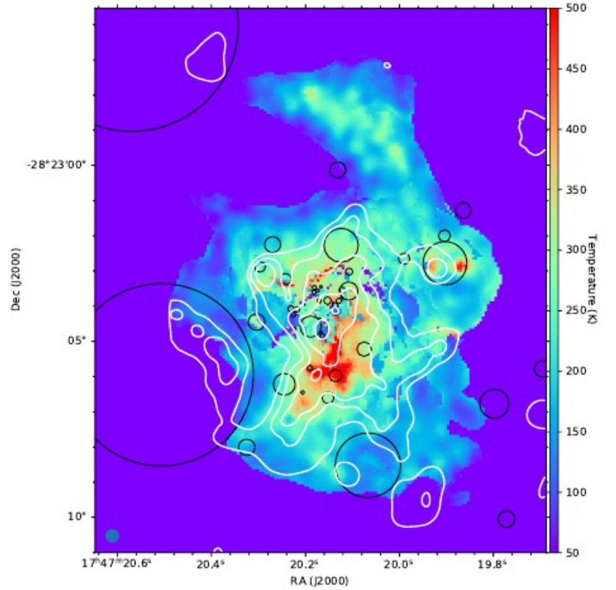
Non-LTE



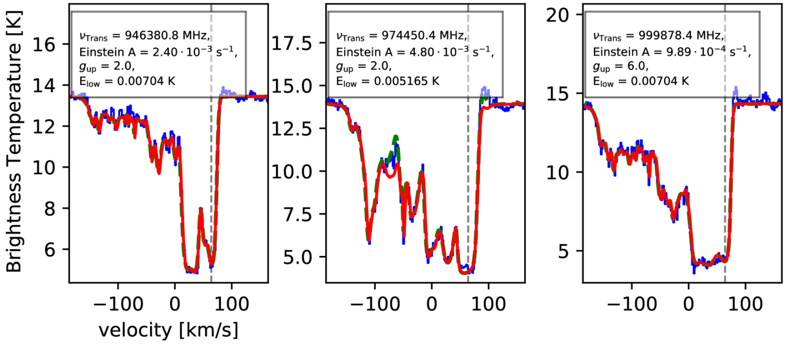


Multi-line LTE fitting





Complex line shape fitting



Physical model fitting

Physical parameter fitting in maps

Automatic optimized fitting using radiative transfer

https://xclass.astro.uni-koeln.de

Data from VAMDC/CDMS

Line catalogue access in IRAM software

iram Institut de Radioastronomie Millimétrique



IPAG Institut de Planétologie et d'Astrophysique de Grenoble

J.Pety, S. Bardeau, E. Reynier,
IRAM

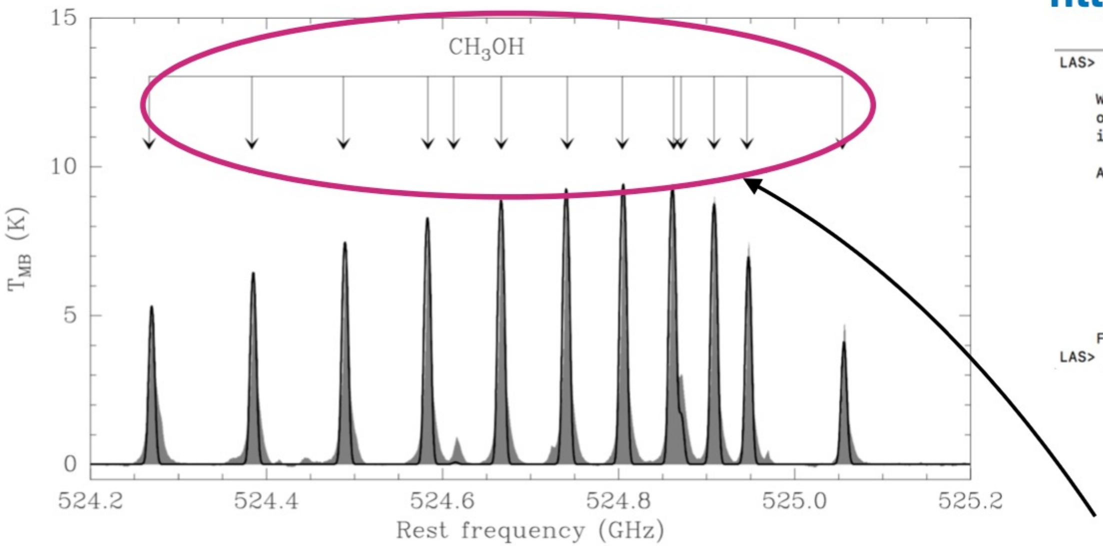
S. Maret, P. Hily-Blant,
IPAG

WEEDS

An extension of the IRAM/CLASS software. It allows for **searches in atomic and molecular lines databases** (e.g. JPL or CDMS) via a **VO-protocol** **Maret, S. et al. , (2011)**

GILDAS SOFTWARE

https://www.iram.fr/IRAMFR/GILDAS/




```
LAS> help weeds\

    Weeds is a CLASS extension to analyze spectral surveys or spectral lines
    observations with large bandwidths.  It  provides  several  commands  to
    identify lines on a spectrum and to model it.

    Available commands:
        LID        Identify lines on the current spectra
        LFIND      Find lines from a species within a frequency range
        LLIST      List lines from the line index
        LGET       Get a line from the line index
        LPLOT      Plot a line from the current line index
        MODSOURCE  Model the emission of a source assuming LTE
        MODSHOW    Show the results of MODSOURCE

    For more information of each command, type 'help <command>'
LAS>
```

IVOA

January 2021

30m radiotelescope - Spain

NOEMA, French Alpes
12 15m antennas

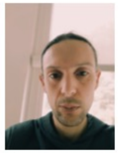
IRAM

Distributed Quick-Look Viewer for IRAM Archive

iram Institut de Radioastronomie Millimétrique


l'Observatoire de Paris | PSL ★ cnrs SORBONNE UNIVERSITÉ

J.Pety, V. De Souza, S. Bardeau, E. Reynier, IRAM




N. Moreau, Y-A Ba, M. Caillat, P. Salomé, LERMA, Observatoire de Paris

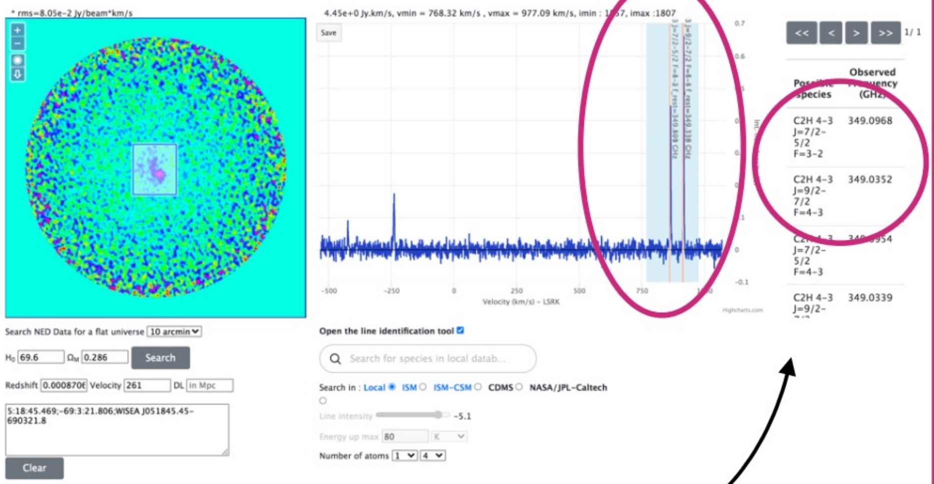
YAFITS@IRAM : Access and visualize IRAM archive (Large Programs) from the web **Quick-Look viewer inside the web-browser**

—> Planned for Early Spring 2022

Using YAFITS : a **distributed Quick-Look** FITS Viewer with **Line identification Tools**

https://yafits.obspm.fr/

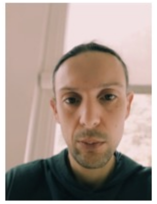
DOI 10.5281/zenodo.3696974



VAMDC consortium **JPL / CDMS databases**

January 2021

ALMA Data Mining and Line identification




N. Moreau, Y-A Ba, M. Caillat, P. Salomé, LERMA, Observatoire de Paris

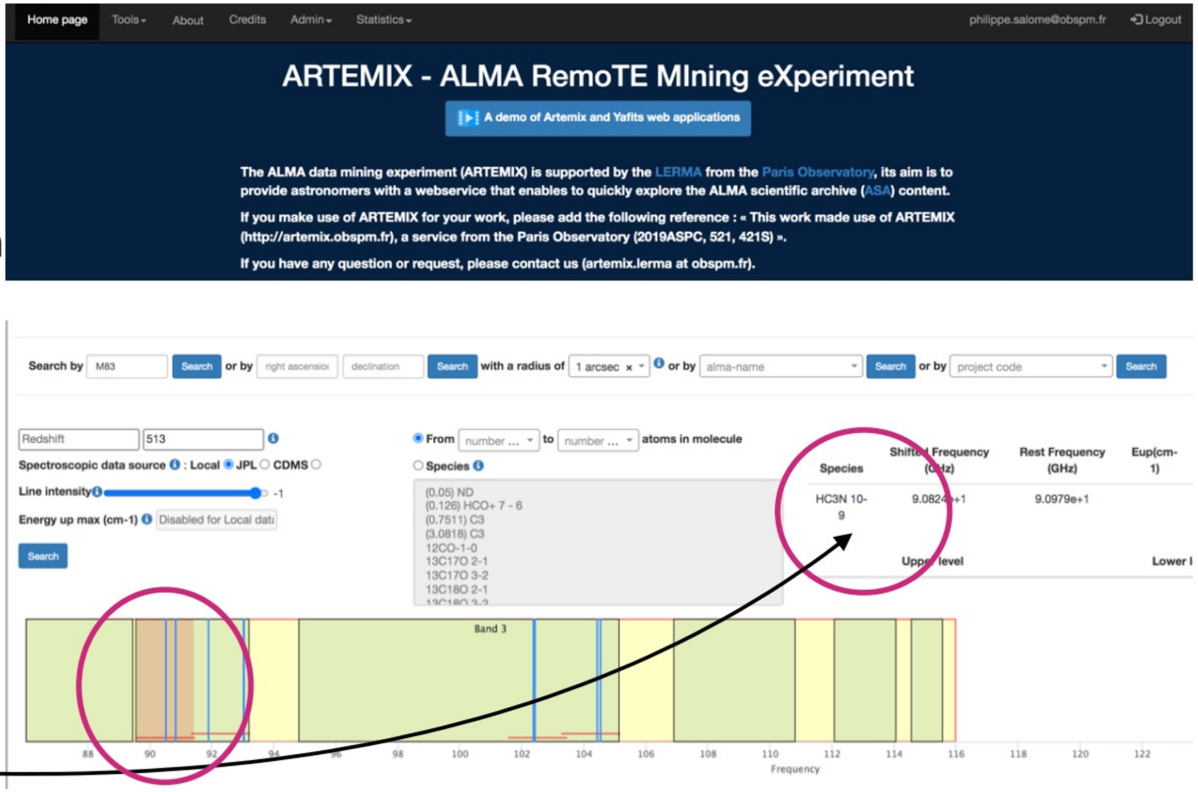
ARTEMIX : a **service to search and display** ALMA data (on-line since 2018).

An experiment for **data mining** the ALMA science Archive, with Line search tools. Also uses **Yafits**

http://artemix.obspm.fr/

VAMDC consortium

JPL / CDMS databases



January 2021

CASSIS Software : http://cassis.irap.omp.eu

- Standalone Software that analyzes and models observations from ground or space-based observatories (mm, sub-mm for now).
- Has implemented VAMDC Queries to spectroscopic data (JPL, HITRAN, CDMS, NIST, etc ..)
- Contact : Charlotte Vastel and Jean-Michel Glorian (Toulouse University, Frce) - Jean-Michel.Glorian@irap.omp.eu, cvastel@irap.omp.eu

Conclusion on VAMDC

- Standards are at the CORE : **Experts** took years to do them
  - They are NOT for the general public, but for the people who implement
- VAMDC standards able to have interoperability at the level of the data
- VAMDC software to operate worldwide (not a central database where different groups put their data)
- Tools offer visibility for different public
  - Portal, standalone GUI : more general public
  - Notebooks : more towards developers
  - User Tools designed by astro. Community
- Connect to other Infrastructure such as IVOA though the Tools (VOTable)

General Conclusion

- Essential InterPlay between Astrophysicists (Observers, Modelers) and Chemical-Physicists/Physicists (experimentalists and theoreticians)
- Tracability of A&M Data is an essential component to reproduce the analysis of observed data and the modelisation of the objects.
- This means that FAIR principles should be used
  - for publishing/Distributing A&M data in databases, portal, e-infrastructures
  - when using those data in analysis software tools and in modeling codes
- The B5 IAU commission will work towards encouraging all those aspects

Aim : A Global Network for Laboratory Astrophysics