

Atomic and Molecular Data in Astrophysics IAU and VAMDC

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

ASOV, France, 11th April 2022

Why Atomic and Molecular Data in Astrophysics ?

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

Different local conditions :

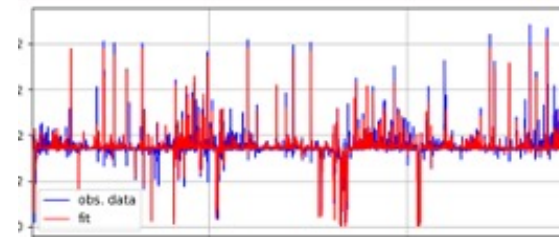
- Temperature and density, Different Species

- 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, VLT, ..)
X (CHANDRA, ATHENA,..)



Astrophysical Spectra
(or images)

Modelisation of the Objects

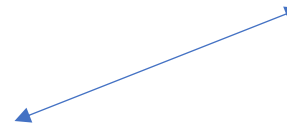
physical model of the object
atomic and molecular processes \leftrightarrow A&M Data

Analysis of Observed Spectra : models object,
radiative transfer methods
atomic and molecular processes \leftrightarrow 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

<i>2-atoms:</i>	AlCl	CP	NaCl	SiN
	AlF	CS	OH	SiO
	AlO	ClH	PN	SiS
	C ₂	FH	PO	SO
	CO	KCl	SiC	TiO
	CN			
<i>3-atoms:</i>	AlOH	CO ₂	H ₂ S	c-SiC ₂
	AlNC	CaNC	HNC	SiCN
	C ₃	FeCN	KCN	SiCSi
	C ₂ H	HCN	MgCN	SiNC
	C ₂ N	HCP	MgNC	
	C ₂ P	H ₂ O	NaCN	TiO ₂
	C ₂ S			
<i>4-atoms:</i>	c-C ₃ H	C ₃ S	H ₂ CS	NH ₃
	ℓ-C ₃ H	C ₂ H ₂	HMgNC	PH ₃
	C ₃ N	HC ₂ N	MgC ₂ H	c-SiC ₃
	C ₃ O	H ₂ CO	NC ₂ P (?)	
<i>5-atoms:</i>	C ₅	CH ₂ CN	HC ₃ N	HNC ₃
	C ₄ H	CH ₄	HC ₂ NC	MgC ₃ N
	C ₄ Si	CH ₂ NH	H ₂ C ₃	SiH ₄
	c-C ₃ H ₂			
<i>6-atoms:</i>	C ₅ H	C ₄ H ₂	HC ₄ N	MgC ₄ H
	C ₅ N	C ₂ H ₄	H ₂ C ₄	SiH ₃ CN
	C ₅ S	CH ₃ CN		
<i>≥ 7-atoms:</i>	C ₆ H	CH ₂ CHCN	HC ₅ N	H ₂ C ₆
	C ₇ H	CH ₃ CCH	HC ₇ N	
	C ₈ H	CH ₃ SiH ₃	HC ₉ N	
<i>Ions:</i>	C ₄ H ⁻	C ₆ H ⁻	C ₈ H ⁻	HCO ⁺
	CN ⁻	C ₃ N ⁻	C ₅ N ⁻	

Some examples

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

OUT OF THIS WORLD

A wealth of molecules is found in interstellar clouds

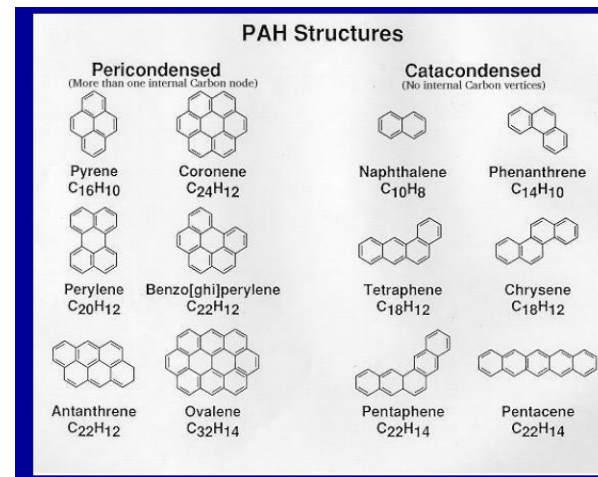
2 atoms	3 atoms	4 atoms	5 atoms
H ₂ NO AlF NS AlCl NaCl C ₂ OH CH PN CH ⁺ SO CN SO ⁺ CO SiN CO ⁺ SiO CP SiS CSi CS HCl HF KCl SH NH FeO	C ₃ MgCN C ₂ H MgNC C ₂ O N ₂ H ⁺ C ₂ S N ₂ O CH ₂ NaCN HCN OCS HCO SO ₂ HCO ⁺ c-SiC ₂ HCS ⁺ CO ₂ HOC ⁺ NH ₂ H ₂ O H ₃ ⁺ H ₂ S SiCN HNC AlNC HNO	c-C ₃ H HNCS l-C ₃ H HOCO ⁺ C ₃ N H ₂ CO C ₂ O H ₂ CN C ₃ S H ₂ CS C ₂ H ₂ H ₂ O ⁺ HCCN NH ₃ HCNH ⁺ SiC ₃ HNCO	C ₅ HC ₂ NC C ₄ H HCOOH C ₄ Si H ₂ CHN l-C ₃ H ₂ H ₂ C ₂ O c-C ₃ H ₂ H ₂ NCN CH ₂ CN HNC ₃ CH ₄ SiH ₄ HC ₃ N H ₂ COH ⁺

6 atoms	7 atoms	8 atoms	9 atoms
C ₅ H CH ₂ SH l-H ₂ C ₄ HC ₃ NH ⁺ C ₂ H ₄ HC ₂ CHO CH ₃ CN NH ₂ CHO CH ₃ CN C ₃ N CH ₃ OH	C ₆ H CH ₂ CHCN CH ₂ CHCN CH ₃ C ₂ H HCN HCOCH ₃ NH ₂ CH ₃ c-C ₂ H ₄ O CH ₂ CHOH	CH ₃ C ₃ N HCOOCH ₃ CH ₂ COOH C ₇ H CH ₂ OHCHO	CH ₃ C ₄ H CH ₃ CH ₂ CN [CH ₃] ₂ O CH ₃ CH ₂ OH HC ₂ N C ₈ H

NOTE: Evidence suggests that much larger molecules such as polycyclic aromatic hydrocarbons and fullerenes are also present.
SOURCE: National Radio Astronomy Observatory

10 atoms	11 atoms	13 atoms
CH ₃ C ₅ N [CH ₃] ₂ CO NH ₂ CH ₂ COOH	HC ₉ N	HC ₁₁ N

Interstellar Medium



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

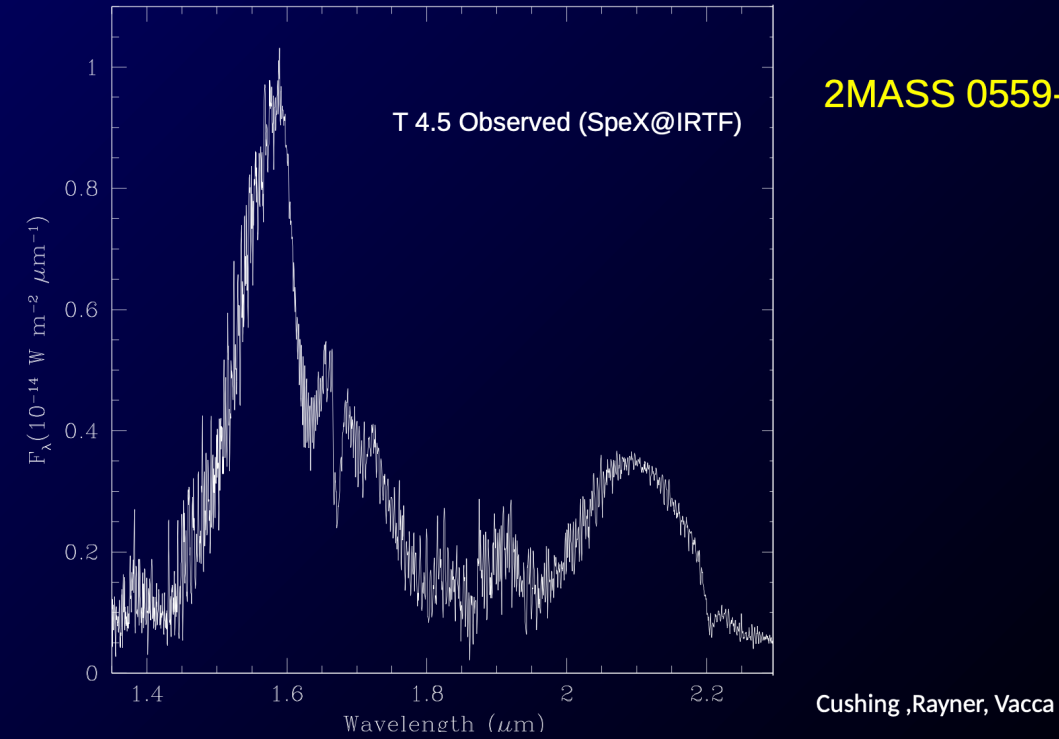
Study of (exo) planets and small objects : what the physical, chemical, dynamical processes underlying the evolution of thoses objects ?

Solar Environnements and plasmas

Periodic Table

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H Hydrogen 1.008																	2 He Helium 4.0026
3 Li Lithium 6.941	4 Be Beryllium 9.0122											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305											13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.06	17 Cl Chlorine 35.45	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.88	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.69	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.63	33 As Arsenic 74.922	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.798
37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.94	43 Tc Technetium 98.906	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.905	46 Pd Palladium 106.34	47 Ag Silver 107.868	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.757	52 Te Tellurium 127.6	53 I Iodine 126.905	54 Xe Xenon 131.29
55 Cs Cesium 132.905	56 Ba Barium 137.327	57 La Lanthanum 138.905	58 Ce Cerium 140.12	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.24	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.50	67 Ho Holmium 164.930	68 Er Erbium 167.259	69 Tm Thulium 168.934	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.967	72 Hf Hafnium 178.49
73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.222	78 Pt Platinum 195.084	79 Au Gold 196.967	80 Hg Mercury 200.59	81 Tl Thallium 204.384	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium 209	85 At Astatine 210	86 Rn Radon 222	87 Fr Francium 223	88 Ra Radium 226	89 Ac Actinium 227	90 Th Thorium 232.038
91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.07	97 Bk Berkelium 247.07	98 Cf Californium 251.08	99 Es Einsteinium 252.083	100 Fm Fermium 257.10	101 Md Mendelevium 258.10	102 No Nobelium 259.10	103 Lr Lawrencium 260.10	104 Rf Rutherfordium 261.10	105 Db Dubnium 262.10	106 Sg Seaborgium 266.10	107 Bh Bohrium 264.10	108 Hs Hassium 277.10
109 Mt Meitnerium 268.10	110 Ds Darmstadtium 271.10	111 Rg Roentgenium 272.10	112 Cn Copernicium 285.10	113 Nh Nihonium 284.10	114 Fl Flerovium 289.10	115 Mc Moscovium 288.10	116 Lv Livermorium 293.10	117 Ts Tennessine 294.10	118 Og Oganesson 294.10								
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137 Bh Bohrium 264.10	138 Hs Hassium 277.10	139 Mt Meitnerium 268.10	140 Ds Darmstadtium 271.10	141 Rg Roentgenium 272.10	142 Cn Copernicium 285.10	143 Nh Nihonium 284.10	144 Fl Flerovium 289.10	145 Mc Moscovium 288.10	146 Lv Livermorium 293.10	147 Ts Tennessine 294.10	148 Og Oganesson 294.10						

Spectrum T4.5 brown dwarf: a “methane dwarf”

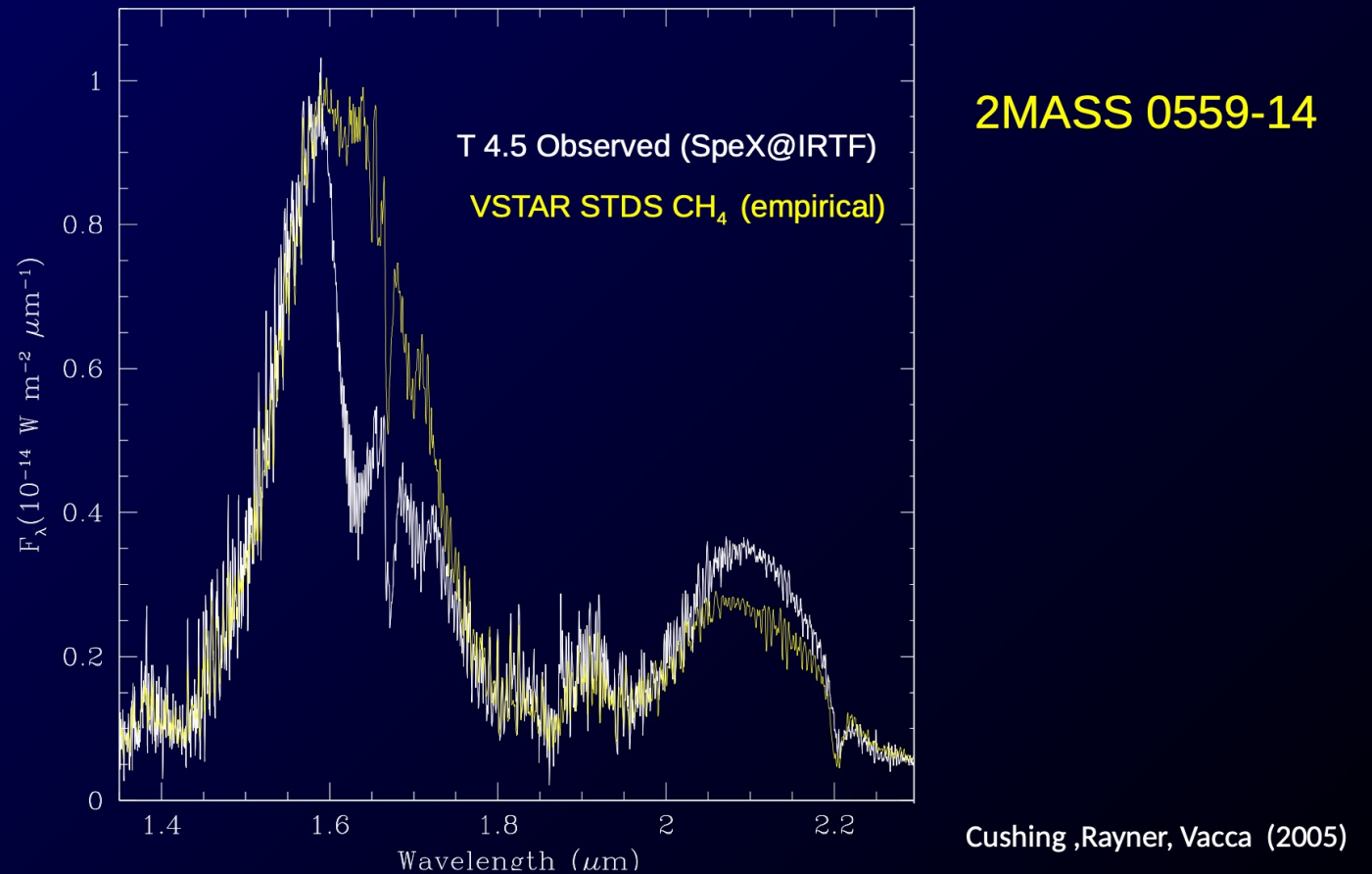


Courtesy of J. Tennyson

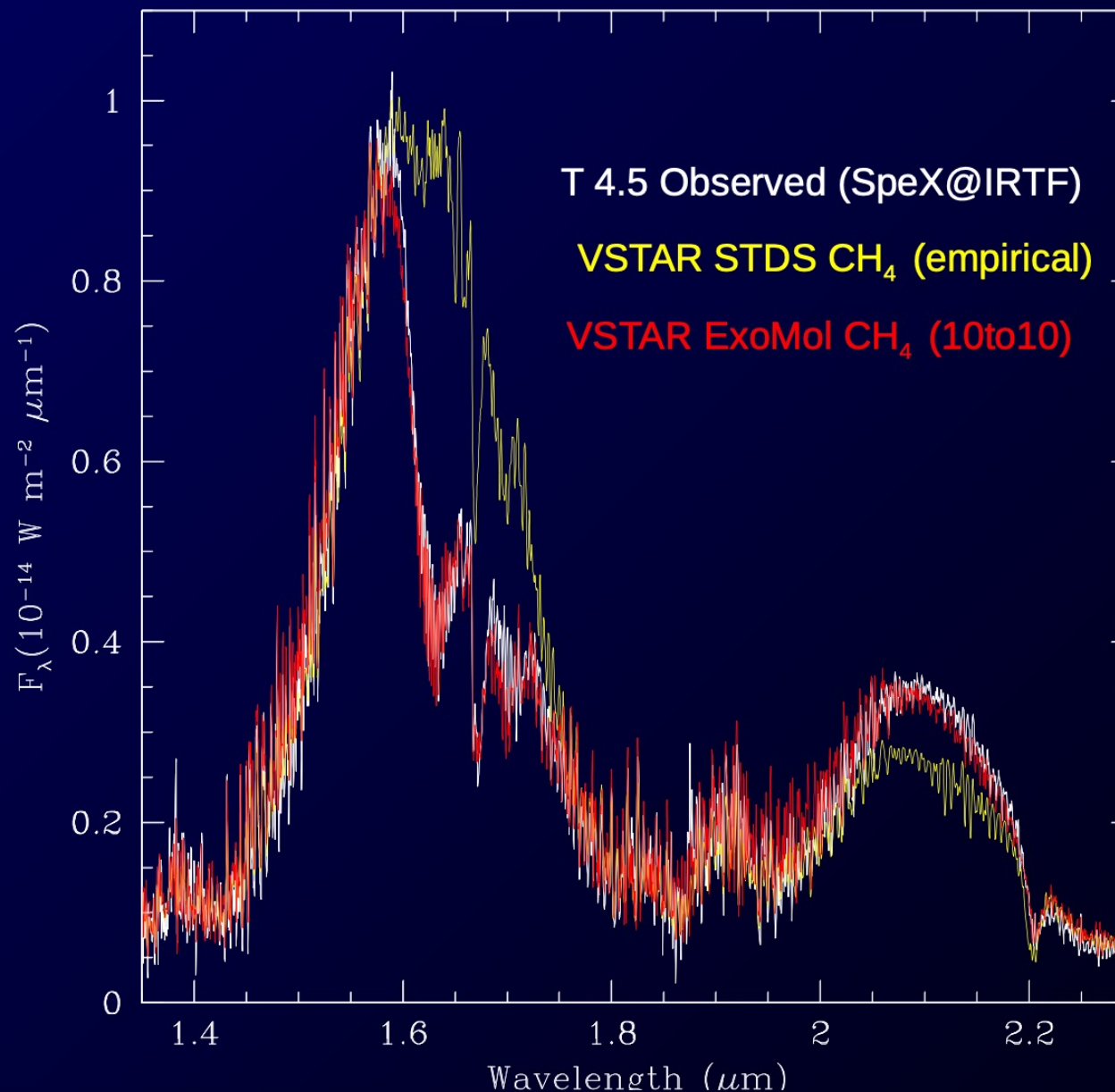
Example of how knowledge on astrophysical object progresses thanks to new calculations that provide more data

Here is the status in 2005

Spectrum T4.5 brown dwarf: a “methane dwarf”



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)

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



B5 IAU Commission (since 2015)

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

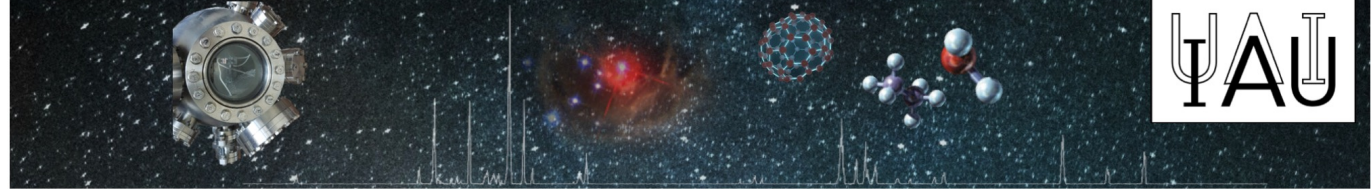
https://www.iau.org/science/scientific_bodies/commissions/B5/

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

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

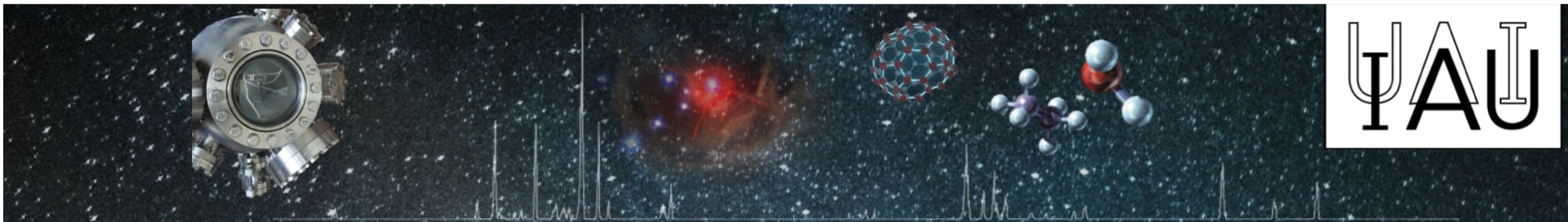
IAU GA B5 commission days, 8th August 2022

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.

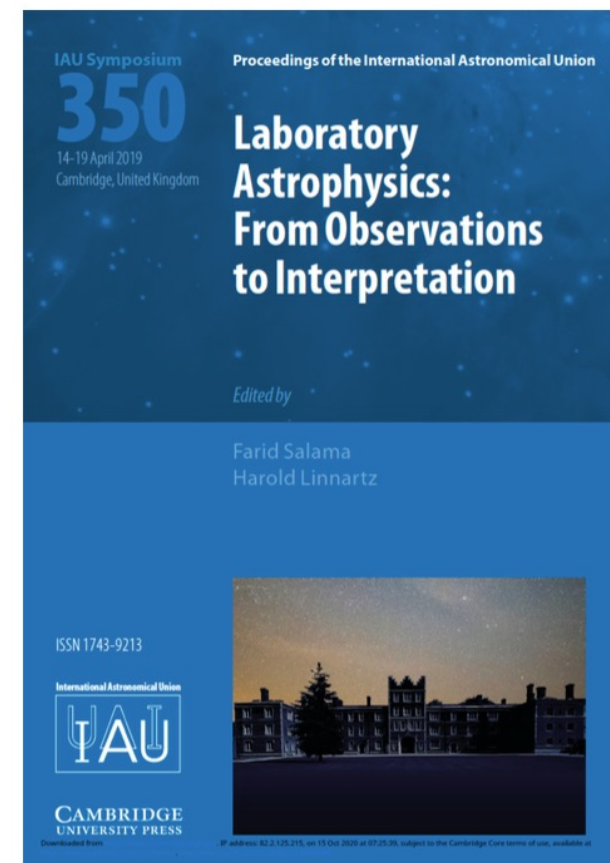


Activities of Commission B5

- 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 Jäger - 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, Netherlands)
- 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

More than
20 years of collaboration

Continued annual
workshops

2020: 8 groups

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

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)

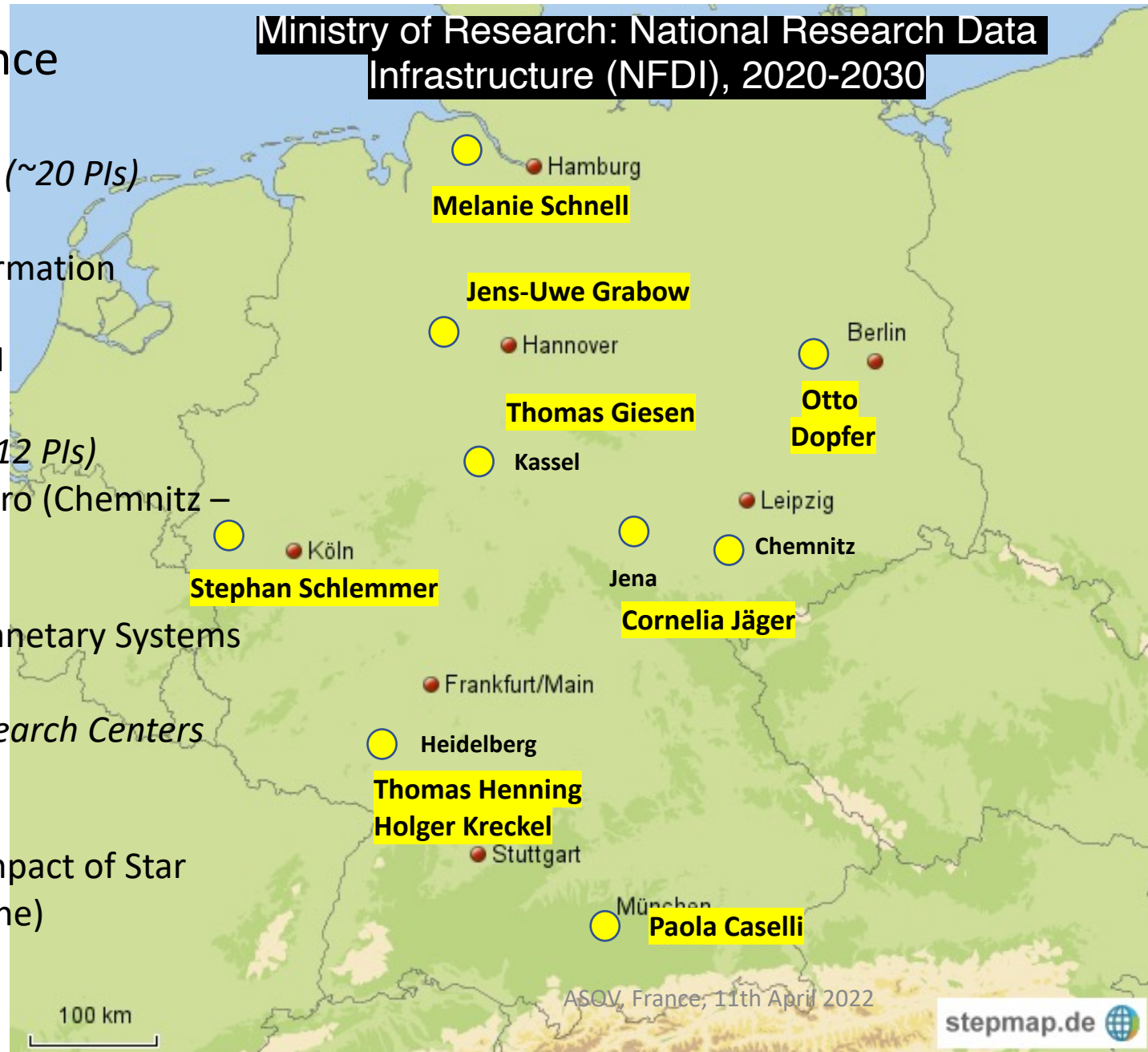
2017-2023

Debris Disks in Planetary Systems

*Collaborative Research Centers
(~15 PIs)*

2011- 2022

Conditions and Impact of Star
Formation (Cologne)



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 Database : snapshots

Astrochem-tools : provided by V. Wakelam

Opacity Project : provided by F. Delahaye

ExoMol : provided by J. Tennyson

LIDA [Leiden Ice Database for Astrochemistry]

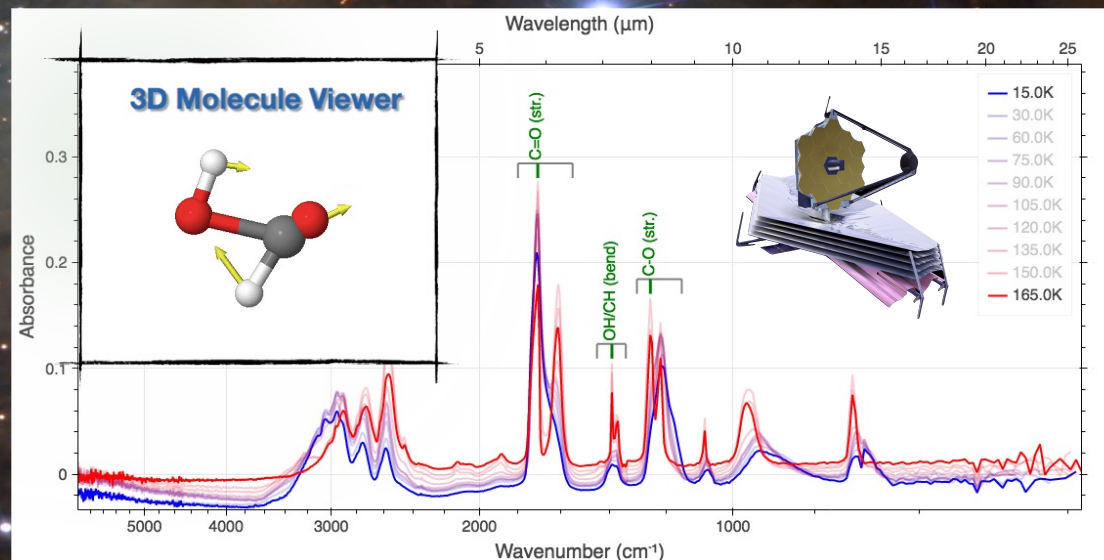
icedb.strw.leidenuniv.nl

Details available soon from Rocha et al. (2022)

Example:
IR spectrum:
HCOOH:



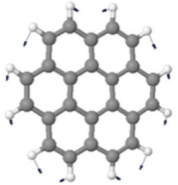
JWST/ERS
ICE AGE



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

ASOV, France, 11th April 2022

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](#)

AmesPAHdbIDL Suite

AmesPAHdbPython Suite

pyPAHdb

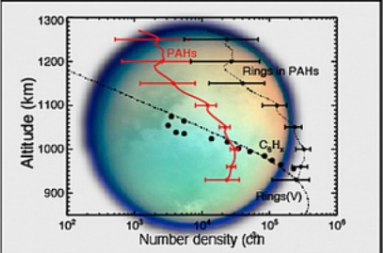
[repository](#)

[repository](#)

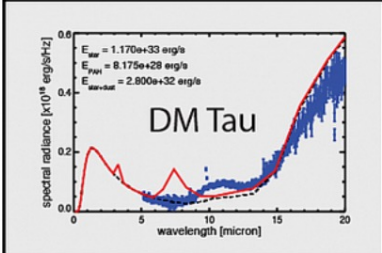
[repository](#)

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".



Solar System



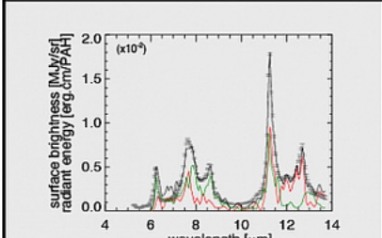
Disks



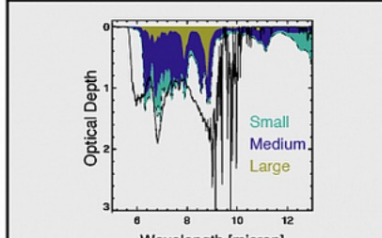
Novae



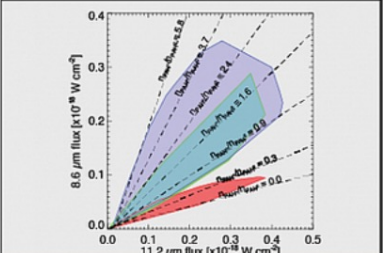
Globules



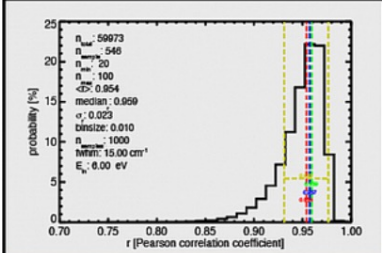
Galaxies



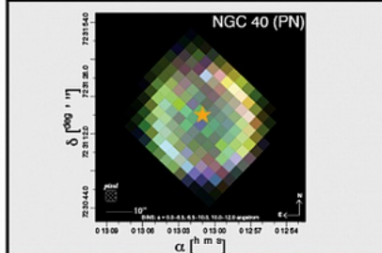
Ices



Proxy Calibration

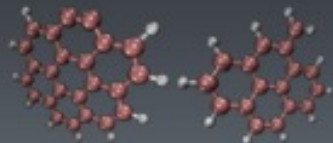


Universal Nature

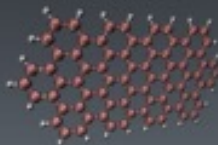


Nebulae

France, 11th



Cosmic PAH portal



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COSMIC PAH portal

[Table of Contents](#)

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.



Osservatorio
Astronomico
di Cagliari





[\(https://astrochem-tools.org/\)](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.



Klnetic Database for Astrochemistry

<http://kida.astrochem-tools.org/>



InterStellar Abundance database

<http://isa.astrochem-tools.org/>



AstroChemical Newsletter

<http://acn.astrochem-tools.org/>



Nautilus gas-grain code

<https://forge.oasu.u-bordeaux.fr/LAB/astrochem-tools/pnautilus>



Astrochemical forum

<https://discourse.astrochem-tools.org/>

Coordinators: Pierre Gratier and Valentine Wakelam



Funding



The Opacity Project: Opacitiy services

<https://opserver.obspm.fr/>

Raw atomic data

TOPbase: Photoionisation Cross Sections

Home

Table of Content

e-levels

f-values

x-sections

QUERY OPTIONS

For the ionic system or range of systems, please indicate
Atomic number (NZ):
Electron number (NE):
Spin multiplicity (2S+1):
Angular momentum (L):
Parity (P, even=0, odd=1):
If you want to be more specific, specify a range of
Levels:
or
Energy (Ryd):
Do you want levels ordered in:
☒ Level order in each series?
☐ General energy order?

OUTPUT OPTIONS

Each level is uniquely identified by its
• Atomic number (NZ)
• Electron number (NE)
• SLPI = (2S+1)*100+L*10+P
• Level index.

Submit Query

Reset

TOPbase: Energy levels

Home

Table of Content

e-levels

f-values

x-sections

QUERY OPTIONS

For the ionic system or range of systems, please indicate
Atomic number (NZ):
Electron number (NE):
Spin multiplicity (2S+1):
Angular momentum (L):
Parity (P, even=0, odd=1):
If you want to be more specific, specify a range of
Levels:
or alternatively
Energy (Ryd):
Do you want levels ordered in:
☒ Level order in each series?
☐ General energy order?

OUTPUT OPTIONS

Each level is uniquely identified by its
• Atomic number (NZ)
• Electron number (NE)
• SLPI = (2S+1)*100+L*10+P
• Level index.
For each level, data to be listed may include
☒ Electron configuration
☒ Energy (Ryd) wrt ionization potential
☐ Statistical weight
☐ Quantum defect
☐ Effective quantum number
☐ Radiative lifetime (s⁻¹)

Submit Query

Reset

Opacities

OP Computations of Rosseland mean opacities

Mass-Fractions

Hydrogen Mass-Fraction (X):
Metal Mass-Fraction (Z):

Metal Fractional Composition (default = 592)

These metal abundances are re-normalized to the value of Z which has been set — it is necessary to specify only the relative abundance for each metal. A negative abundance implies that the element is included in the mixture but its opacity is excluded.

C (Z=6)	0.2460	N (Z=7)	0.0647	O (Z=8)	0.5140
Ne (Z=10)	0.0815	Na (Z=11)	0.00148	Mg (Z=12)	0.02636
Al (Z=13)	0.00205	Si (Z=14)	0.0246	S (Z=16)	0.01125
Ar (Z=18)	0.0023	Ca (Z=20)	0.00159	Cr (Z=24)	0.000324
Mn (Z=25)	0.00017	Fe (Z=26)	0.02244	Ni (Z=28)	0.00123

Output options

OPACs and their derivatives for a given temperature-density mesh. The mesh can be specified by a range or a tabulation of (log(T), log(ρ)) or (log(T), log(ρ)) where T is the temperature in Kelvin, ρ the density in g cm⁻³ and Rlog(T)² with T_{eff}=1.6.4.
Please choose ONE of the following output options:
☒ An intermediate opacity file that can then be used locally for interpolation (temperature-density) with the code `opht tar go`
☐ (log(T), log(ρ))
☐ (log(T), log(ρ))
☐ Local file with tabulation of (log(T), log(ρ))
☐ Local file with tabulation of (log(T), log(ρ))
☐ Local file with tabulation of (log(T), log(ρ))
☐ Local file with tabulation of (log(T), log(ρ))

Number of points: 10
Log Scale: 0.5
Email address:

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The Opacity Project

The Iron Project

TOPbase

TIPbase

OPserver

OP tables

Contact

OP The Opacity Project

The name Opacity Project (OP) [1] refers to an international collaboration that was formed in 1984 to calculate the extensive atomic data required to estimate stellar envelope opacities and to compute Rosseland mean opacities and other related quantities. It involved research groups from France, Germany, the United Kingdom, the United States and Venezuela. The approach adopted by the OP to calculate opacities is based on a new formalism of the equation of state [2] and on the computation by ab initio methods of accurate atomic properties such as energy levels, f-values and photoionization cross sections [3]. The OP final results are discussed by Seaton et al. [4].
OP opacities have been recently revised to include inner-shell contributions [5]. The new data and a suite of easy-to-use codes to compute Rosseland means and radiative accelerations [6] can be downloaded as a tar file below.
• **Opacity Tables:** Ensembles of opacity tables for specific (pre-determined) composition using The Opacity Project data. The tables are in the OPAL format and can be used in stellar structure and evolutionary codes. All the routines already in stellar evolutionary codes using OPAL tables will work with these tables (under construction).
• **OPCD 3.3:** Tar file (600 Mb) to be downloaded with complete package (data, codes, OPserver and instructions) for computing Rosseland mean opacities and radiative accelerations. Data files are the same as OPCD 2.0, but new software is included to install OPserver at the user's facilities (12-12-06).

The Iron Project - The Opacity Project

IPOPv2

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The Opacity Project

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The Opacity Project - The Iron Project

The names Opacity Project (OP) and Iron Project (IP) refer to an international collaboration that was formed in 1984 to calculate the extensive atomic data required to estimate stellar envelope opacities and to compute Rosseland mean opacities and other related quantities. It involved research groups from France, Germany, the United Kingdom, the United States and Venezuela. The approach adopted by the OP to calculate opacities is based on a new formalism of the equation of state and on the computation by ab initio methods of accurate atomic properties such as energy levels, f-values and photoionization cross sections. The OP final results are discussed by Seaton et al.

Badnell Nigel, Ballance Connor, Bautista Manuel, Butler Keith, Delahaye Franck, Del Zanna Giulio, Eissner Werner, Fivet Vanessa, Hudson Claire, Kang Guiyun, Mason Helen, McLoughlin Brendan, Mendoza Claudio, Montenegro Max, Nahar Sultana, Palmeri Patrick, Pradhan Anja, Quinet Pascal, Ramsbottom Cathy, Saraph Hannelore, Scott Penny, Storey Peter, Wason Ian, Witthoft Mike, Zeppen Claude,

Links

AstroAtom blog
Databases for Atomic and Plasma Physics - W.I.S.
ADAS
CHIANTI
Atomic & Plasmas physic db
Members only
Next Meeting
Previous Meeting
Activities

Atm. Data db

κ_P, κ_R

κ_V Spectral db

Next: Experimental measurements!

Provided by F. Delahaye

ASOV, France, 11th April 2022

23

I. BeH, MgH, CaH

II. SiO

III. HCN/HNC

IV. CH₄

V. NaCl, KCl

VI. PN

VII. PH₃

VIII. H₂CO

IX. AlO

X. NaH

XI. HNO₃

XII. CS

XIII. CaO

XIV. SO₂

XV. HOOH

XVI. H₂S

XVII. SO₃

XVIII. VO

XIX. H₂¹⁸O, H₂¹⁷O

XX. H₃⁺

Hot line lists; Published in MNRAS

XXI. NO

XXII. SiH₄

XXIII. PO, PS

XXIV. SiH

XXV. SiS

XXVI. SN, SH

XXVII. AlH

XXVIII. C₂H₄

XXIX. CH₃Cl

XXX. H₂¹⁶O

XXXI. C₂

XXXII. TiO

XXXIII. MgO

XXXIV. PH

XXXV. NH₃

XXXVI SH (UV)

XXXVII HCCH

XXXVIII SiO₂

XXXIX CO₂

XL. H₃O⁺

XLI. NaOH, KOH

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)

1. Line lists
2. Cross-sections
3. Partition functions
4. Broadening parameters
(Barton et al, JQSRT **187**, 453 & 203, 490 (2017))
H₂ 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

The screenshot shows the Zenodo website interface. At the top, the URL is `https://zenodo.org/search?page=1&size=20&q=VAMDC`. The Zenodo logo is on the left, followed by a search bar containing 'VAMDC'. Navigation links for 'Upload' and 'Communities' are next to the search bar. On the right, there are 'Log in' and 'Sign up' buttons.

Below the header, the search results are displayed. On the left side, there are three filter panels:

- Access Right:** A checkbox for 'Open (42)' is shown.
- File Type:** Checkboxes for 'Zip (24)', '(9)', and 'Pdf (9)' are shown.
- Keywords:** Checkboxes for 'VAMDC (2)', 'Accounting (1)', 'Astronomical Spectroscopy (1)', 'Authentication (1)', 'Authorisation (1)', and 'Databases (1)' are shown.

The main content area shows 'Found 42 results.' with a pagination bar (1, 2, 3) and a 'Sort by:' dropdown menu set to 'Best match' and 'asc.'. Three results are visible:

- June 23, 2020 (v1)** | Presentation | Open Access
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
View
- May 1, 2015 (1.0)** | Project deliverable | Open Access
Authentication, Authorisation and Accounting strategy
Zwölf; Rixon;
Authentication, Authorisation and Accounting strategy for the VAMDC infrastructure.
Uploaded on July 9, 2020
View
- April 10, 2018 (2017-01-30)** | Dataset | Open Access
VAMDC extraction with identifier = f29e648a-7c00-4ff7-afe5-5cff38891a3d
VAMDC, Consortium;
View

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

**EUROPEAN OPEN
SCIENCE CLOUD**

All resour... 

My EOSC Marketplace

[Resources](#) > [Processing & Analysis](#) > [Data Management](#) > [Discovery](#) > [VAMDC Portal](#)



VAMDC Portal


A centralized query interface for the whole VAMDC infrastructure
Organisation: [Virtual Atomic and Molecular Data Centre](#)

☆☆☆☆☆ (0.0 / 5) 0 reviews ☐ Add to comparison ☐ Add to favourites

[Webpage](#) [Helpdesk e-mail](#) [Manual](#) [Training information](#) [Ask a question about this resource?](#)

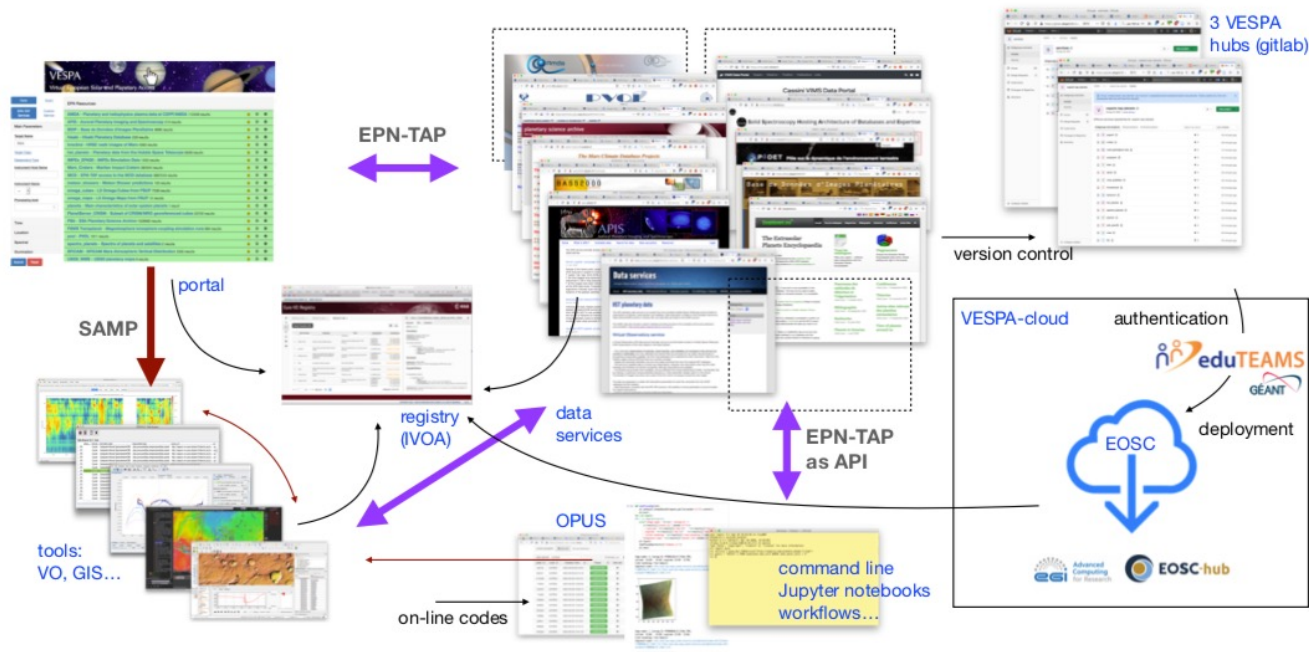
[ABOUT](#) [DETAILS](#) [REVIEWS \(0\)](#)

VAMDC aims to be an interoperable e-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 this portal. It is a unified interface to query multiple databases simultaneously thanks to standardized request language and data format. This service provides a way to query many atomic and molecular services simultaneously. Moreover, as the results share the same data format, it makes it easier to cross-match the results.

SCIENTIFIC CATEGORISATION

Natural Sciences

VESPA from EuroPlanet : imbedding SSHADE

VESPA: infrastructure



Solid Spectroscopy Hosting Architecture of Databases and Expertise



Write your keywords here or leave it empty to get all the data...

Search spectra

Search band lists

Search bands

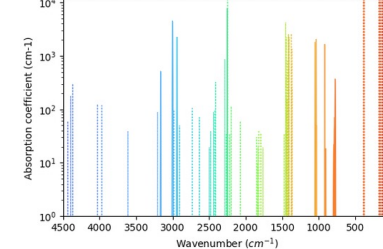
Search publications

News

< > @sshade_eu

New bandlist dataset released: sshade.eu/data/BANDLIST... Absorption band list of CH₃CN in natural solid CH₃CN (phase beta) | BANDLIST database pic.twitter.com/hKC9P7NdBn

Absorption band list of CH₃CN in natural solid CH₃CN (phase beta)



by SSHADE: Databases for Solid Spectroscopy, 2021-12-05 14:10:26 UTC+0000

<https://www.sshade.eu/>



Virtual Atomic and Molecular Data Center - VAMDC

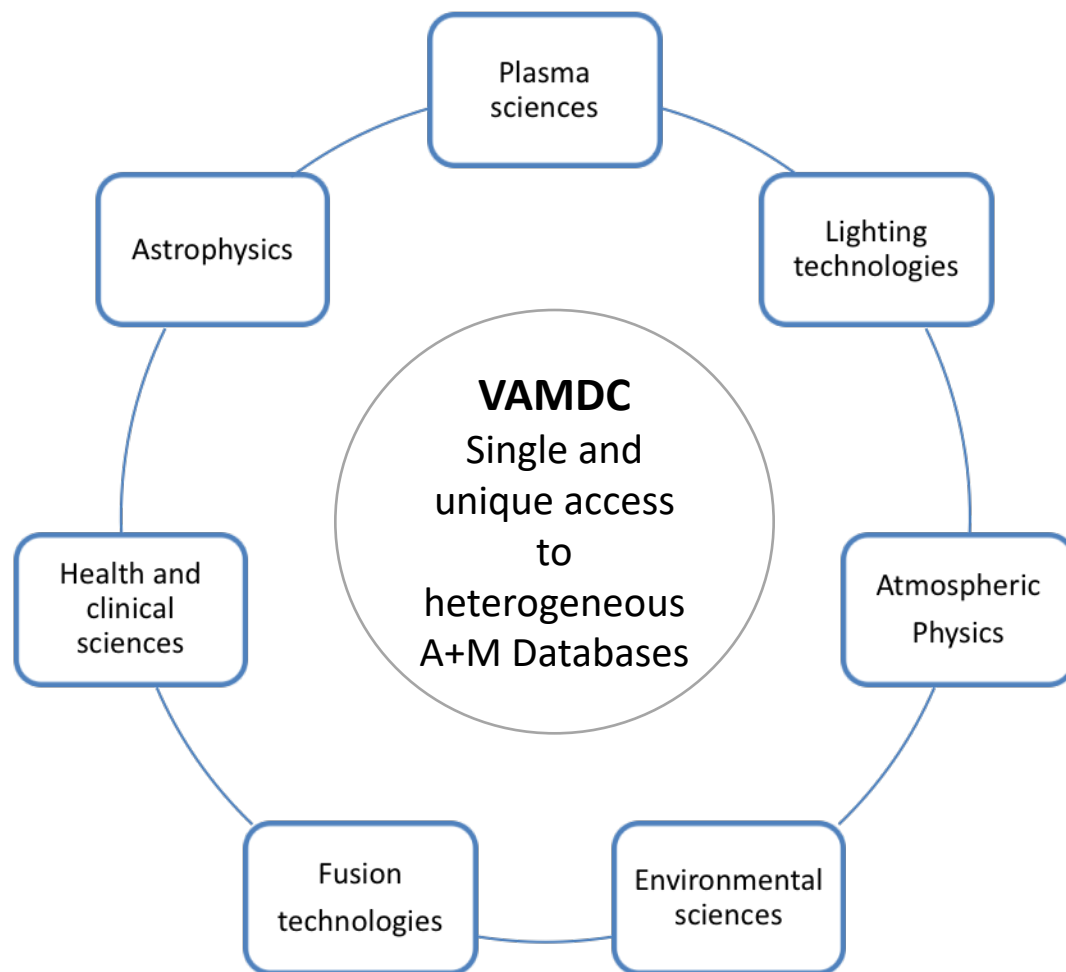
<http://www.vamdc.org>

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

Databases	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-Bréchet	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 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 Marinković	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 ₂ O 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 ₂ H 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, Bangalore, India	Astrophysics, Other
AMBDAS	Collisions in plasmas (bibliographic) - searchable via processes and 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

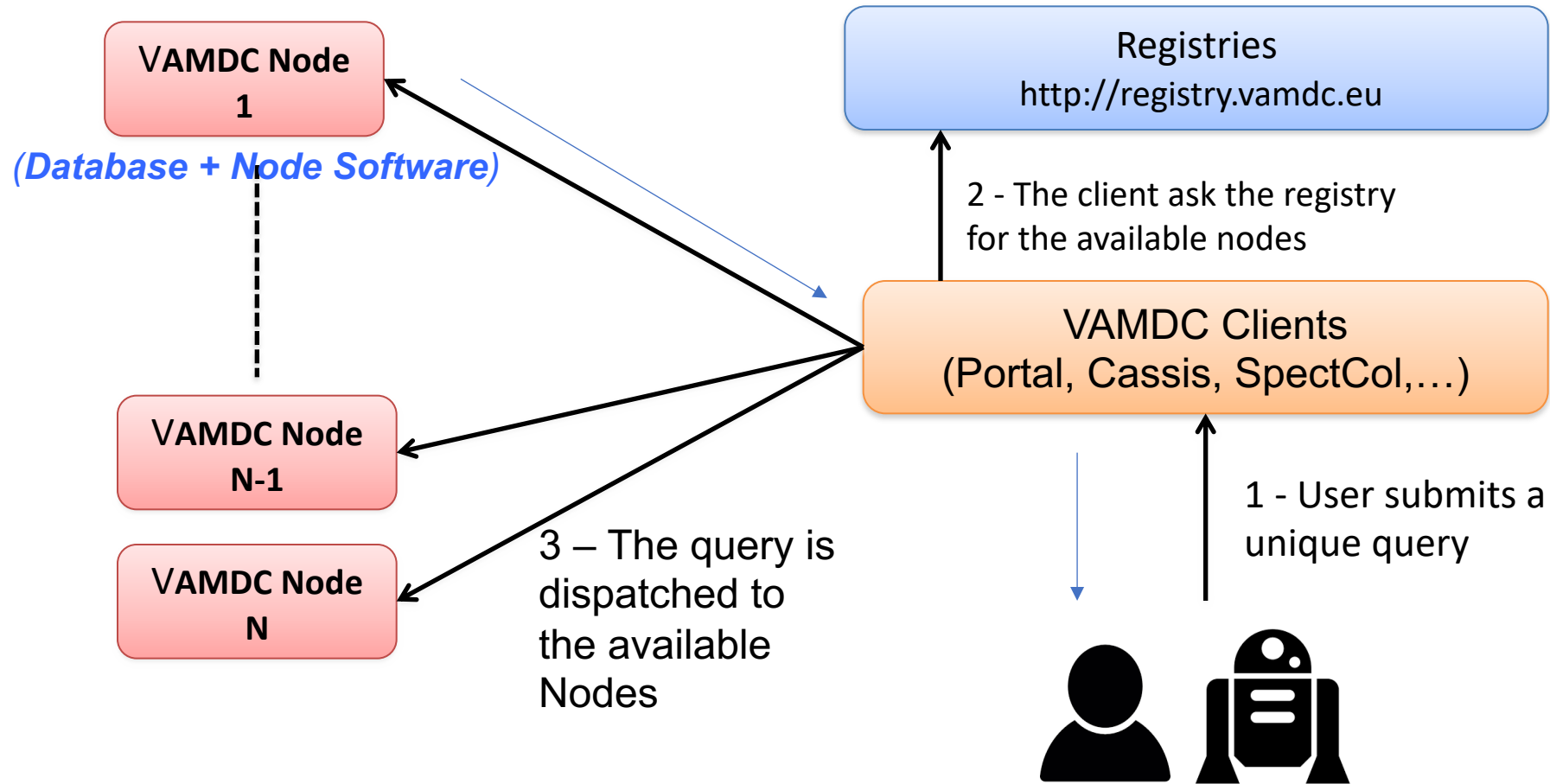
FAIR (Findability, Accessibility, Interoperability, Reuse) principles underlined the design of VAMDC

- **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 Infrastructure

- 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



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**

Data Description : XSAMS format

XML **S**chema for **A**toms **M**olecules and **S**olids

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



20/25 Groups



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



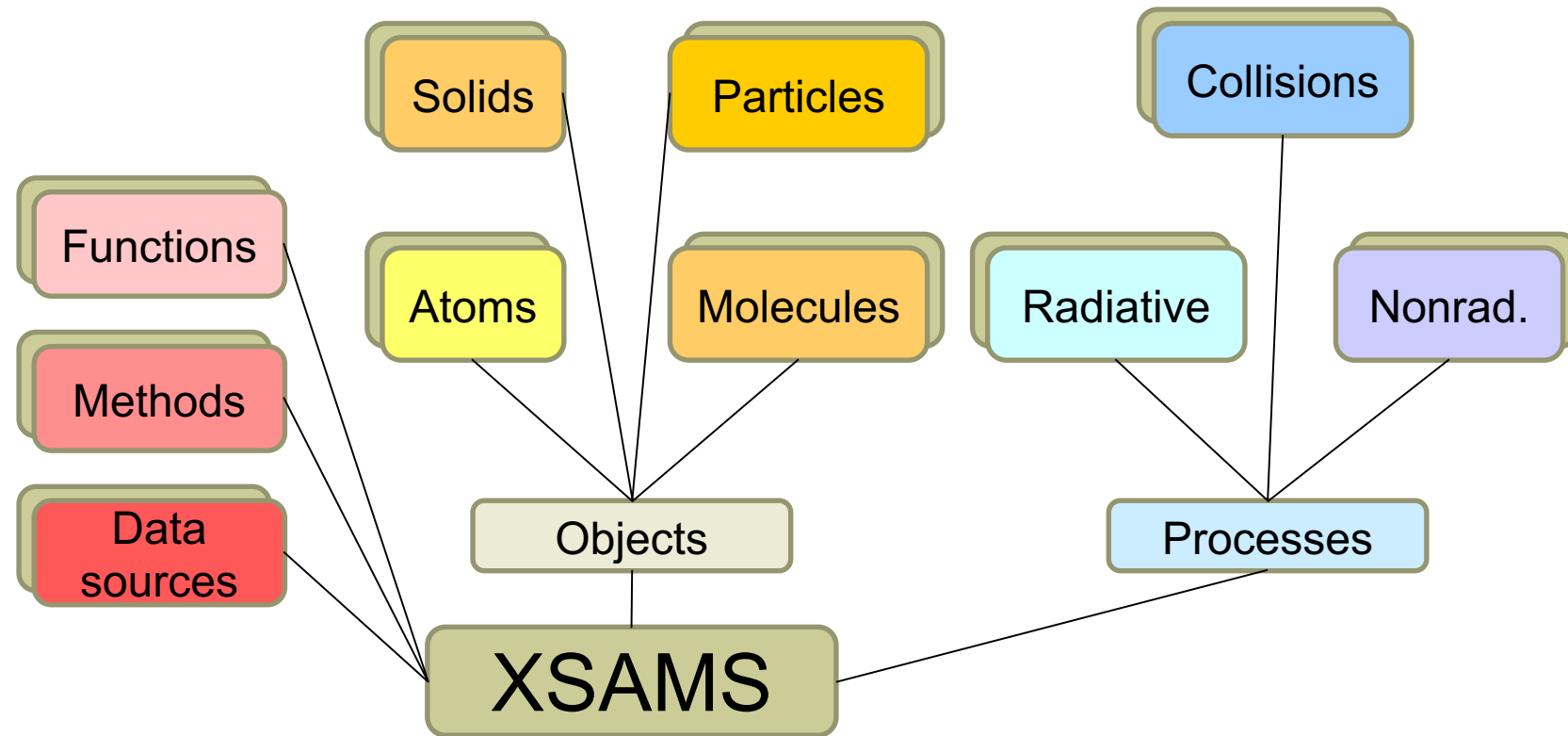
Y. Ralchenko

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



Dictionnaires 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

Restrictables

- AsOfDate
- AtomMass
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- AtomNuclearCharge
- AtomNuclearSpin
- AtomStateCoupling
- AtomStateHyperfineMomentum
- AtomStateIonizationEnergy
- AtomStateKappa
- AtomStateLandeFactor
- AtomStateMagneticQuantumNumber
- AtomStateParity
- AtomStatePolarizability
- AtomStateQuantumDefect
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- AtomSymbol
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- EnvironmentSpeciesPartialPressure
- EnvironmentTemperature
- EnvironmentTotalNumberDensity
- EnvironmentTotalPressure
- FunctionID
- FunctionName
- Inchi
- InchiKey
- IonCharge
- MethodCategory
- MoleculeChemicalName
- MoleculeMolecularWeight

VAMDC Tools

Portal

SPECTCOL Tool

Species Database

Query Store

Bibliographic Service (in development)

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Query by...

Species
 Processes
 Environment
 Advanced

Molecule 1
 [Clear](#)
[Remove form](#)

Chemical name

Stoichiometric formula

Structural formula

Spin isomer

Standard InChIKey

[Select All](#)
[None](#)
 Search by stoichiometric formula if no isotopologue is selected.

Isotopologue
<input type="checkbox"/> Carbon oxide isotopologue $^{18}\text{C}^{18}\text{O}$
<input type="checkbox"/> Carbon oxide isotopologue $^{14}\text{C}^{14}\text{O}$
<input type="checkbox"/> Carbon oxide isotopologue $^{13}\text{C}^{13}\text{O}$
<input type="checkbox"/> Carbon Monoxide $^{13}\text{C}^{18}\text{O}$
<input checked="" type="checkbox"/> CO $^{12}\text{C}^{16}\text{O}$
<input type="checkbox"/> Carbon oxide isotopologue CO-17
<input type="checkbox"/> Carbon oxide isotopologue $^{14}\text{C}^{18}\text{O}$
<input type="checkbox"/> Carbon oxide isotopologue $^{13}\text{C}^{17}\text{O}$

[Find data](#)
[Reset](#)

Legend

available, can answer
available, don't support query
unsupported keyword

- Belgrade electron/atom(molecule) database (BEAMDB)
- TFMeCaSDa - CF₄ Calculated Spectroscopic Database
- GeCaSDa: Gemane Calculated Spectroscopic Database
- KIDA: Kinetic Database for Astrochemistry - TAP service
- Theoretical spectral database of polycyclic aromatic hydrocarbons
- Photodissociation - MolD database
- Chianti
- GSMA Reims S&MPO
- ECaSDa - Ethene Calculated Spectroscopic Database
- NIST Atomic Spectra Database
- GhoSST
- SHeCaSDa - SF₆ Calculated Spectroscopic Database
- Stark-b
- JPL database: VAMDC-TAP service
- HITRANonline
- VALD sub-set in Moscow (obs)
- MeCaSDa - Methane Calculated Spectroscopic Database
- VALD (atoms)
- VAMDC species-DB

TABLE of Databases answering the « CO » request

Query Execution

Done

Modify query

Stop waiting

Save query

Comments

Your request

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

Visualization

Results by node								
Name	Database last update	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
SpEctroScopy of Atoms and Molecules	04/2019 00:00	XSAMS file	1	1459	2000	2000	0	0
Water internet Accessible Distributed Information System	5/11/2015 19:00	XSAMS file	1	320	1000	1000	0	0
CDMS	14/11/2016 14:00	XSAMS file	2	188	182	182	0	0

✓ -- Choose display --

Collisional data XSAMS to HTML

XSAMS to Hitran

BibTeX from XSAMS

Table views of XSAMS

Xsams2SME

Atomic spectroscopy XSAMS to HTML

Molecular spectroscopy XSAMS to HTML

XSAMS multiplexor

-- Choose display --

OK

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%2Fvamd%2Fcdms%2Fvamd-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%2Fvamd%2Fcdms%2Fvamd-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%2Fvamd%2Fcdms%2Fvamd-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%2Fvamd%2Fcdms%2Fvamd-tap_12.07
BCDMS-1920		private communication : 52nd Okaz Okaz	Evenson, K. M.;	1995	http://xsams-processors.obspm.fr/applyXSL
BCDMS-1921	CDMS database	di			
BCDMS-2709	The Cologne Database for Molecular Spectroscopy, CDMS, in the Virtual Atomic and Molecular Data Centre, VAMDC	journal : J. (Vol : 327 95 , Pa			

Results from CDMS VAMDC node

Unselect all	Chemical name X	Stoichiometric formula X	Ord stru for
--------------	-----------------	--------------------------	--------------

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
<input checked="" type="checkbox"/>	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
<input checked="" type="checkbox"/>	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
<input checked="" type="checkbox"/>	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
<input checked="" type="checkbox"/>	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
<input checked="" type="checkbox"/>	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
<input checked="" type="checkbox"/>	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
<input checked="" type="checkbox"/>	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
<input checked="" type="checkbox"/>	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
<input checked="" type="checkbox"/>	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
<input checked="" type="checkbox"/>	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
<input checked="" type="checkbox"/>	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
<input checked="" type="checkbox"/>	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
<input checked="" type="checkbox"/>	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
<input checked="" type="checkbox"/>	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
<input checked="" type="checkbox"/>	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

Using the

Molecular spectroscopy XSAMS to HTML

visualisation

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)



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

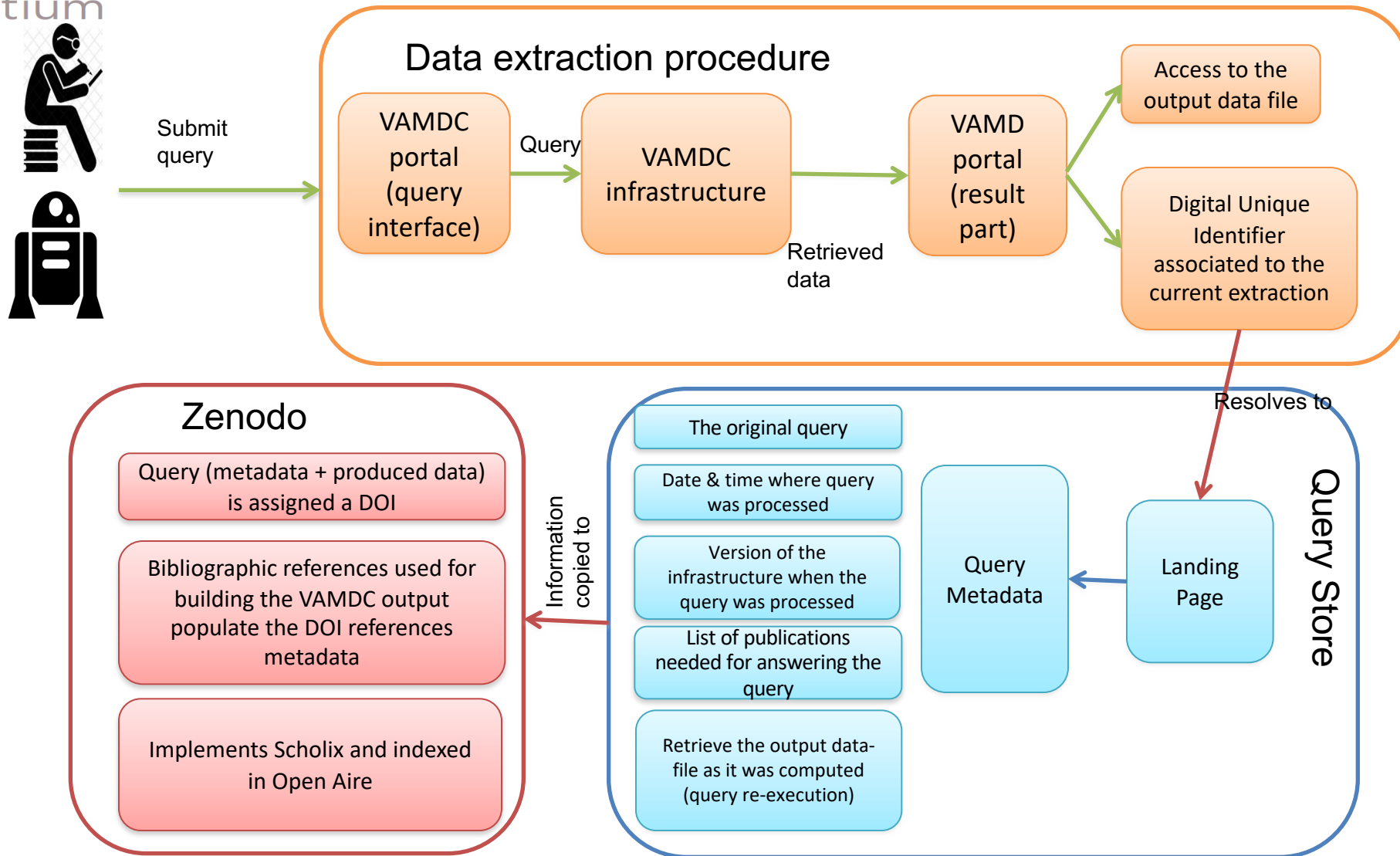
[TIPbase : VAMDC-TAP interface](#) (Atomic states, Atoms, Collisions)

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

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

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

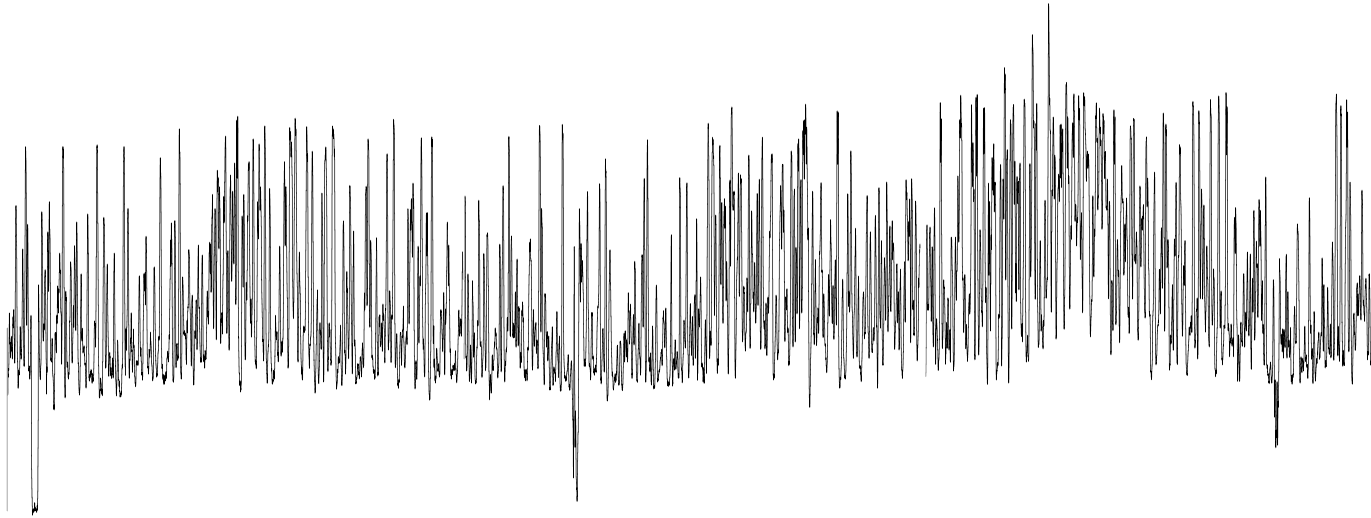
XCLASS (Cologne, Provided by P. Schilke)

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

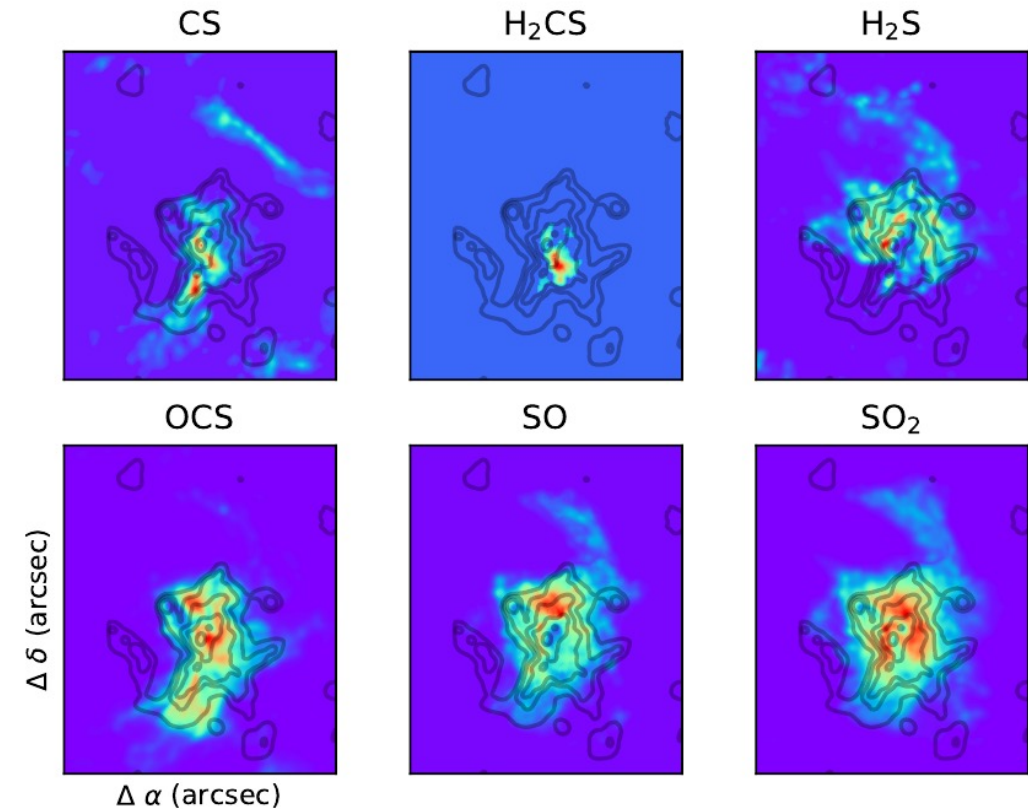
CASSIS (Toulouse, re-organised information from materials from J.M. Glorian)

ASTROPHYSICS SOFTWARE TOOLS (A&M EMBEDDED) –

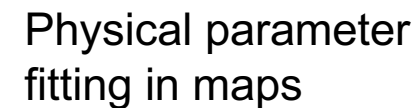
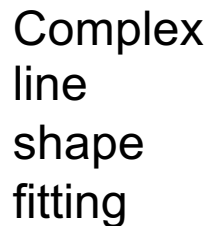
Challenge: analysis of complex spectra and maps



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



(P. Schilke and coll)



Automatic optimized fitting using radiative transfer
<https://xclass.astro.uni-koeln.de>
Data from VAMDC/CDMS

Line catalogue access in IRAM software



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



Institut de Planétologie et
d'Astrophysique de Grenoble

S. Maret, P. Hily-Blant,
IPAG



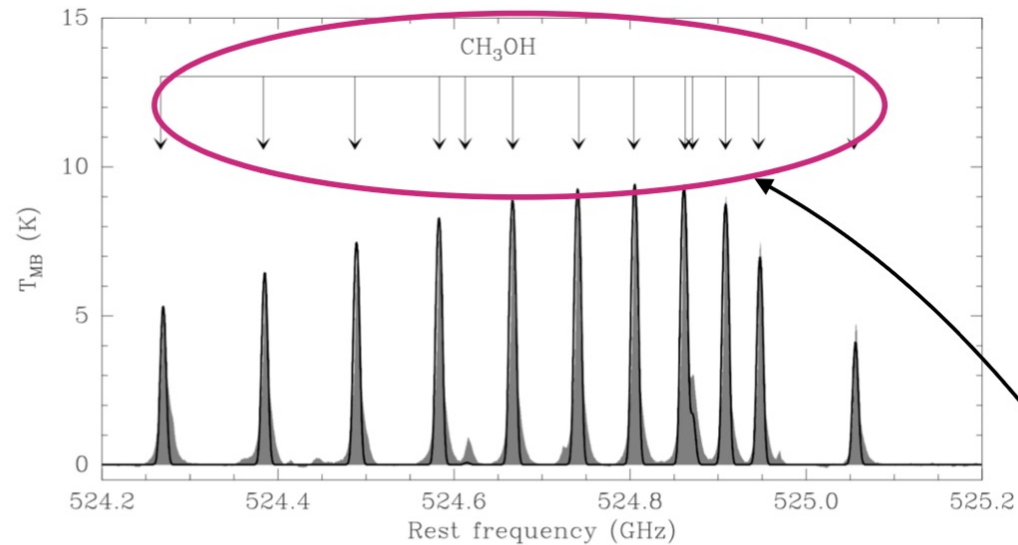
30m radiotelescope - Spain

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)



<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> █



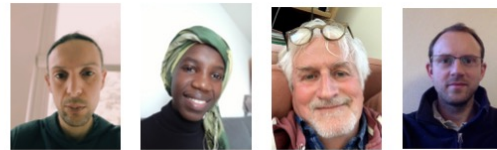
NOEMA, French Alps
12 15m antennas

IRAM

Distributed Quick-Look Viewer for IRAM Archive



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



Large Programs

IRAM offers the possibility to apply for observing time in the framework of a Large Program using NOEMA and the 30-meter telescope. Please consult the current [Call for Proposals](#) as different restrictions may apply for both observatories during a given observing semester.

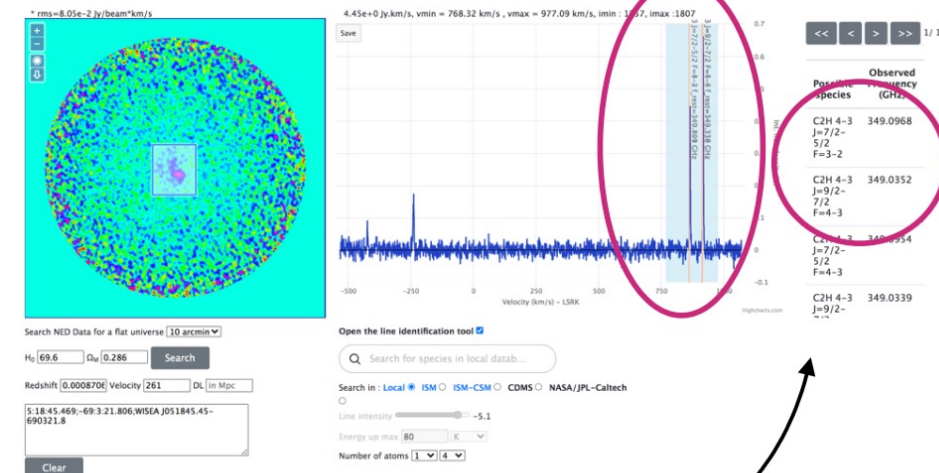
Please consult the [Large Program Policy](#) for more details.

A comprehensive summary of completed and on-going (standard) Large Programs can be found in the [IRAM Data Archive](#).

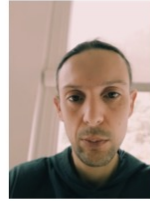
The MPG-IRAM Observatory Programs (MIOP) started first observations during autumn 2019 and is run under LP policy with special source protection. More details are given [here](#).

Using YAFITS : a **distributed Quick-Look** FITS Viewer with **Line identification Tools**
<https://yafits.obspm.fr/>

DOI 10.5281/zenodo.3696974



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/>



JPL / CDMS databases

Home page Tools About Credits Admin Statistics philippe.salome@obspm.fr Logout

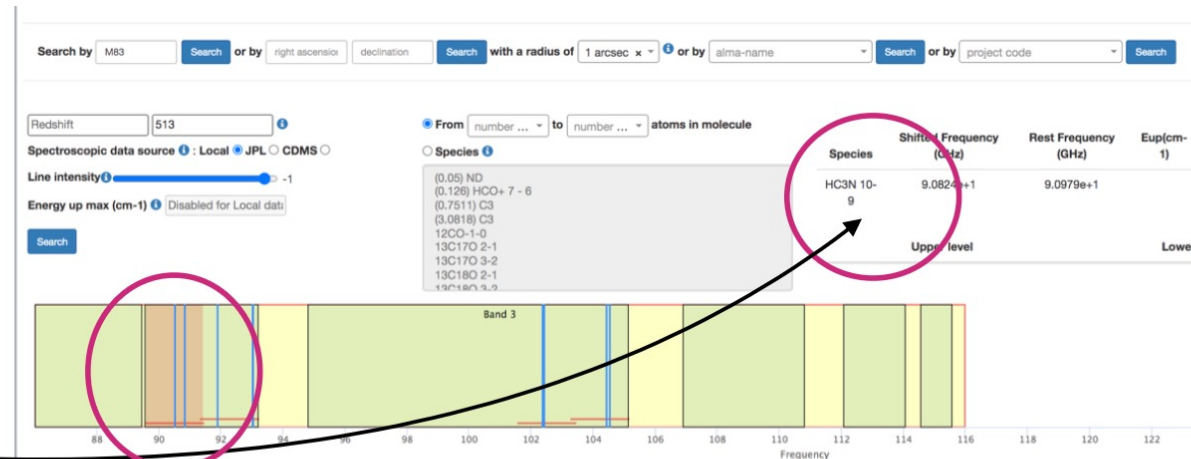
ARTEMIX - ALMA RemoTE Mining eXperiment

[A demo of Artemix and Yafits web applications](#)

The ALMA data mining experiment (ARTEMIX) is supported by the **LERMA** from the Paris Observatory, its aim is to provide astronomers with a webservice that enables to quickly explore the ALMA scientific archive (**ASA**) content.

If you make use of ARTEMIX for your work, please add the following reference : « This work made use of ARTEMIX (<http://artemix.obspm.fr>), a service from the Paris Observatory (2019ASPC, 521, 421S) ».

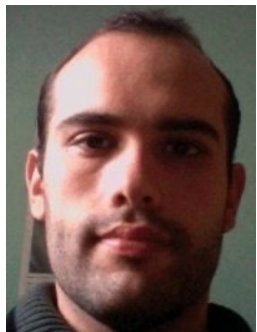
If you have any question or request, please contact us (artemix.lerma@obspm.fr).



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, France) - 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