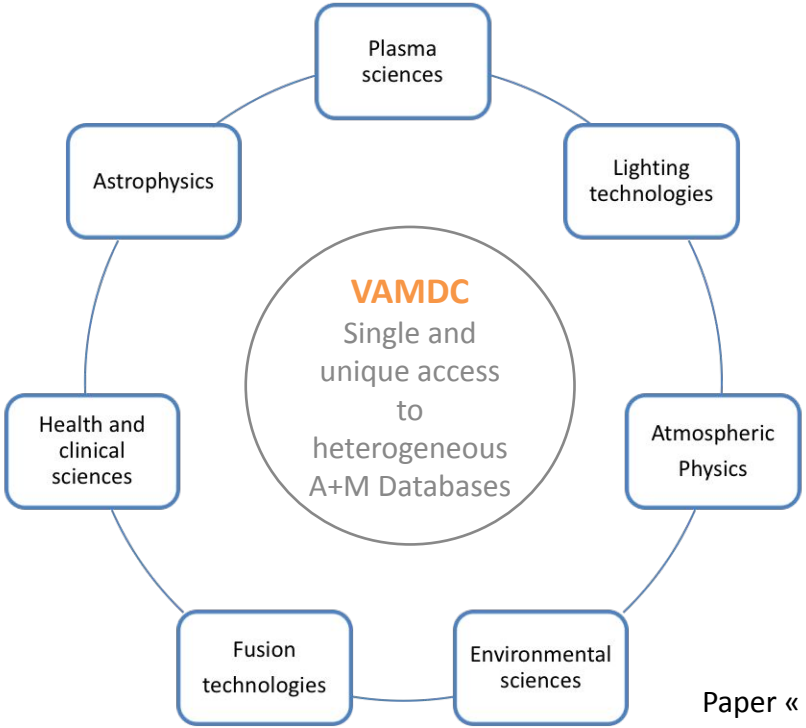
The pyVAMDC library

ASOV 2025 - 24/03/2025

Carlo Maria Zwölf, Nicolas Moreau

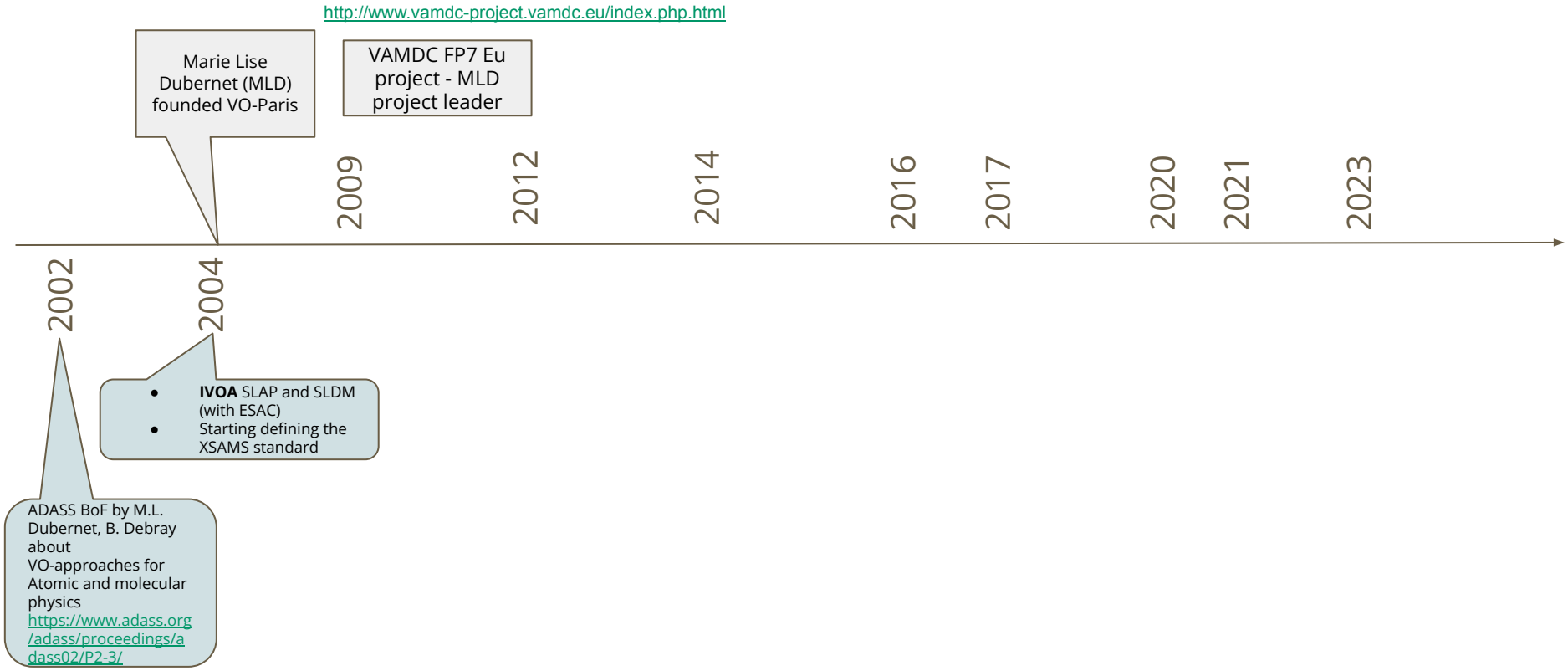
The Virtual Atomic and Molecular Data Centre in a nutshell



- E-infrastructure connecting about 40 heterogeneous databases (*Nodes*) that can be accessed from http://portal.vamdc.org/ or any VAMDC compatible tools
- Consortium of 25 partners
- High quality scientific data come from different Physical/Chemical Communities
- Provides a large dissemination platform to data producers
- **Interoperability of queries and output**

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

Perspective of a long ongoing process



Perspective of a long ongoing process

http://www.vamdc-project.vamdc.eu/index.php.html

Marie Lise Dubernet (MLD) founded VO-Paris

VAMDC FP7 Eu project - MLD project leader

2002 2004 2009 2012 2014 2016 2017 2020 2021 2023

ADASS BoF by M.L. Dubernet, B. Debray about VO-approaches for Atomic and molecular physics https://www.adass.org/adass/proceedings/adass02/P2-3/

- **IVOA** SLAP and SLDM (with ESAC)
- Starting defining the XSAMS standard

- First version of portal
- Species database (for internal usage, manually fed)
- VAMDC Registry, using Astrogrid solutions

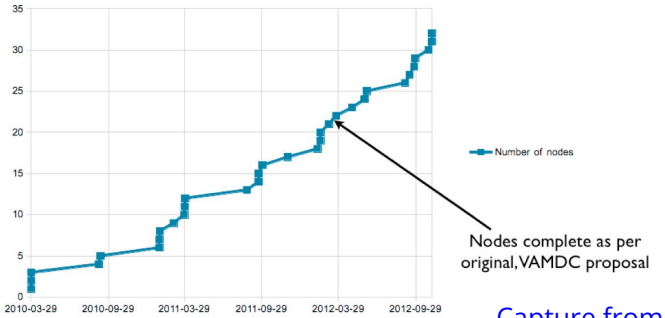
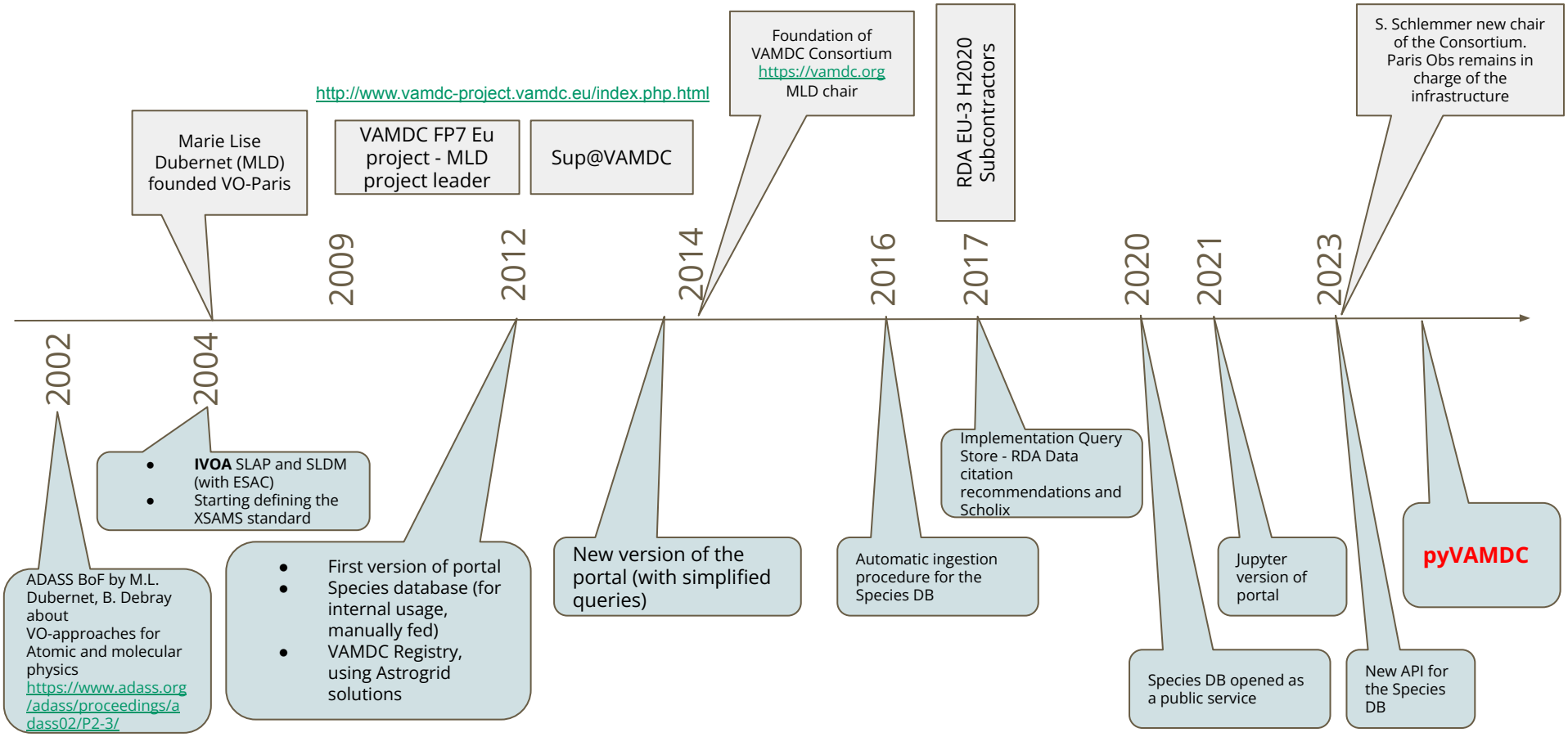


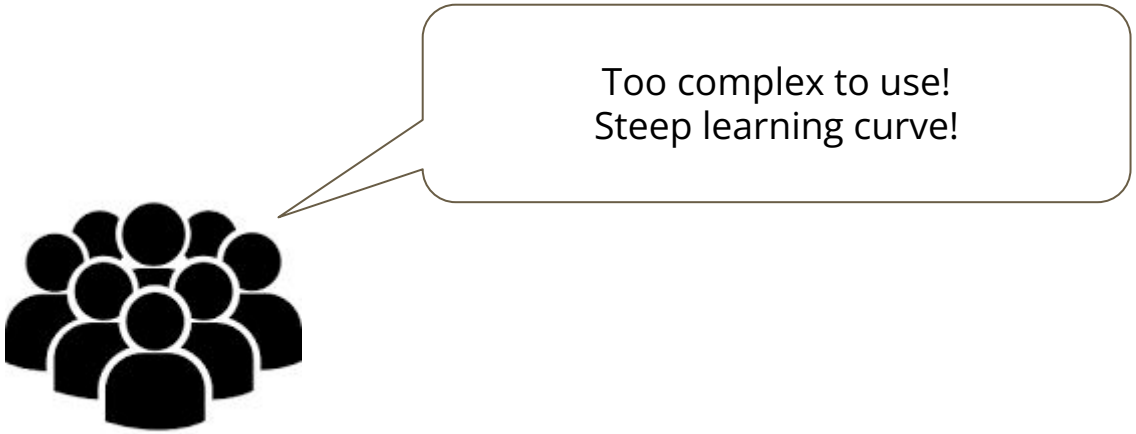
Figure 1: growth of VAMDC infrastructure, by count of data nodes

Capture from WP4 4.5 vamdc project delivrable

Perspective of a long ongoing process



VAMDC is nice, but…



VAMDC is nice, but...

Too complex to use!
Steep learning curve!

pyVAMDC

```
1 import pyVAMDC.spectral.lines as lines
2 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max)
```

https://github.com/VAMDC/pyVAMDC/

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That’s it. Thank you for your attention…

A deeper look to pyVAMDC

```
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A deeper look to pyVAMDC

Optional fields

```
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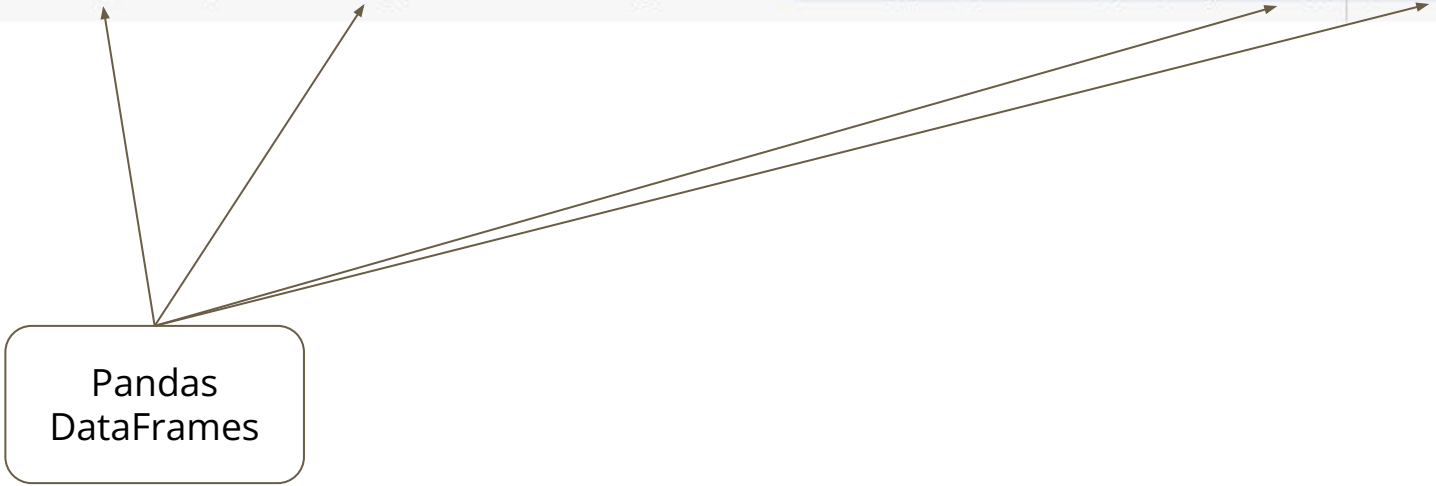

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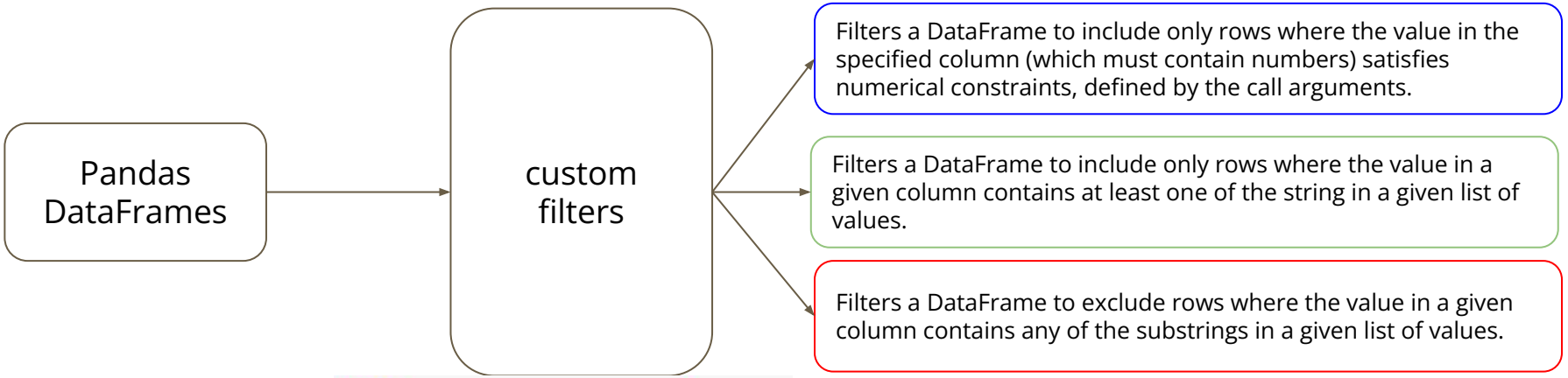


```
import pyVAMDC.spectral.filters as filters
```

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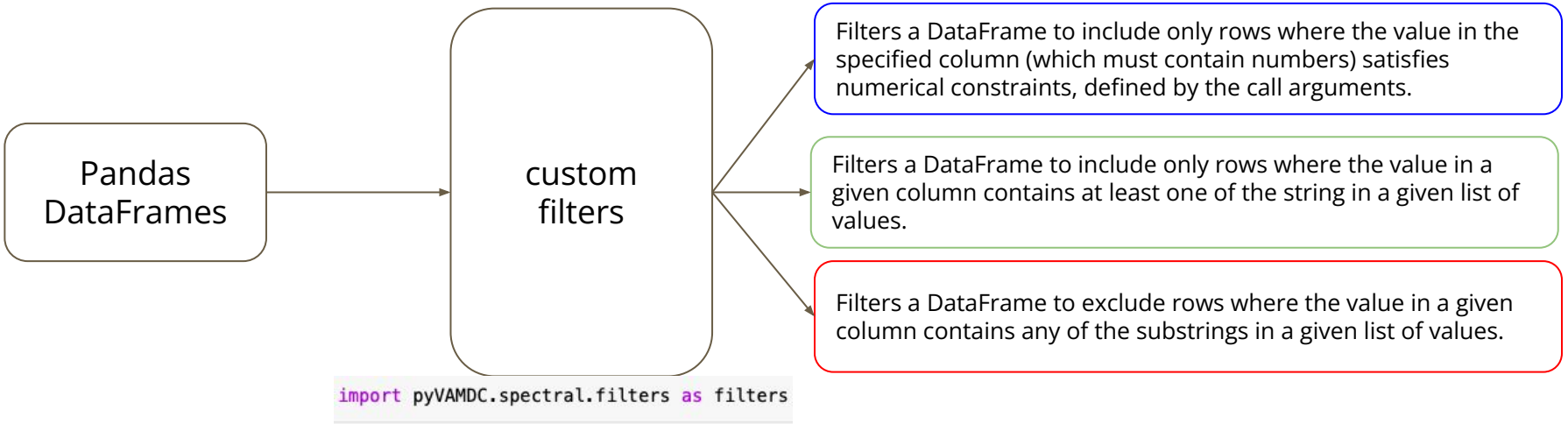

Don’t even need to know Pandas’ syntax!!

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1 to 25 of 32 entries Filter

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2	AMDIS Ionization		emoto.masahiko@nifs.ac.jp	ivo://vamdc/amdis-ionization	http://dbshino.nifs.ac.jp:4000/vamdc/tap/	https://dbshino.nifs.ac.jp/nifsdb/	2025-02-12 15:47:44	2025-02-12||2025-02-12	Atomic states,Atoms,Collisions
0	Acetylene Spectroscopic Databank 1000K (VAMDC-TAP)		vip@iao.ru roman2400@rambler.ru	ivo://vamdc/asd-1000	http://lts.iao.ru/node/asd-1000/tap/	ftp://ftp.iao.ru/pub/	2025-02-12 15:47:44	2025-02-12||2025-02-12	Molecular states,Molecules,Radiative transitions
3	BASECOL2015: VAMDC-TAP interface		yaye-awa.ba@obspm.fr	ivo://vamdc/basecol2015/vamdc-tap	http://basecoltap2015.vamdc.org/12_07/TAP/	https://basecol.vamdc.org/	2025-02-12 15:47:44	2025-02-12||2025-02-12	Atomic states,Atoms,Collisions,Molecular states,Molecules
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index	shortName	ivoIdentifier	inChI	inChIKey	stoichiometricFormula	massNumber	charge	speciesType	structuralFormula	name	did	tapEndpoint	lastIngestionScriptDate	speciesLastSeenOn	# unique atoms	# total atoms	computed charge	computed mol_weight
4584	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/C7HN/c1-2-3-4-5-6-7-8/h1H	XRJCSTPFBZTAPK-UHFFFAOYSA-N	C7HN	99	0	molecule	HCCCCCCCN	Cyanohexatriyne, Cyanotriacetylene	XRJCSTPFBZTAPK-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	3.0	9.0	0.0	99.010899032
4585	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/ClNO3/c1-5-2(3)4/i1+2	XYLGPCWDPLOBGP-NJFSPNSNSA-N	ClNO3	99	0	molecule	Cl-37-ONO2	Chlorine nitrate	XYLGPCWDPLOBGP-NJFSPNSNSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	3.0	5.0	0.0	98.95372045
4586	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/C7O/c1-2-3-4-5-6-7-8	ARYJKUMSSIOOOH-UHFFFAOYSA-N	C7O	100	0	molecule	C7O	Heptacarbon monoxide	ARYJKUMSSIOOOH-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	8.0	0.0	99.99491462
4587	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/Cl2O2/c1-3-4-2	MAYPHUUCLRDEAZ-UHFFFAOYSA-N	Cl2O2	Not provided	0	molecule	ClOOCl	Chlorine peroxide	MAYPHUUCLRDEAZ-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	4.0	0.0	101.9275346
4588	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/Cl2O2/c1-2-4-3	NKVCUZORVXMYQU-UHFFFAOYSA-N	Cl2O2	Not provided	0	molecule	ClClO2	Chloryl chloride	NKVCUZORVXMYQU-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	4.0	0.0	101.9275346
4589	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/Cl2O2/c1-3-4-2/i1+2	MAYPHUUCLRDEAZ-NJFSPNSNSA-N	Cl2O2	104	0	molecule	Cl-37-OOCl	Chlorine peroxide	MAYPHUUCLRDEAZ-NJFSPNSNSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	4.0	0.0	103.92458451
4590	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/BrO2/c2-1-3/i1-1	SISAYUDTHCIGLM-BJUDXGSMSA-N	BrO2	Not provided	0	molecule	OBr-79-O	Bromine dioxide	SISAYUDTHCIGLM-BJUDXGSMSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	3.0	0.0	110.90816634000001
4591	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/C8O/c1-2-3-4-5-6-7-8-9	XNKLVPGGOLSCFA-UHFFFAOYSA-N	C8O	112	0	molecule	C8O	Octacarbon monoxide	XNKLVPGGOLSCFA-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	9.0	0.0	111.99491462
4592	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/O2Se/c1-3-2/i3+1	JPJALAQPGMAKDF-LBPDFUHNSA-N	O2Se	112	0	molecule	Se-80-O2	Selenium dioxide	JPJALAQPGMAKDF-LBPDFUHNSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	3.0	0.0	111.90635054
4593	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/BrO2/c2-1-3/i1+1	SISAYUDTHCIGLM-OUBTZVSYSA-N	BrO2	113	0	molecule	OBr-81-O	Bromine dioxide	SISAYUDTHCIGLM-OUBTZVSYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	3.0	0.0	112.90611984
4594	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/C9O/c1-2-3-4-5-6-7-8-9-10	ZUGKIQCRTZHRDF-UHFFFAOYSA-N	C9O	124	0	molecule	C9O	Nonacarbon monoxide	ZUGKIQCRTZHRDF-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	10.0	0.0	123.99491462
4595	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/S4/c1-3-4-2	IOOGPFMMGKCAGU-UHFFFAOYSA-N	S4	Not provided	0	molecule	S4	Tetrasulfur, Cyclo-tetrasulfur	IOOGPFMMGKCAGU-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	1.0	4.0	0.0	127.888284
4596	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/IO/c1-2	AFSVSXMRDKPOEW-UHFFFAOYSA-N	IO	Not provided	0	molecule	IO	Iodine monoxide	AFSVSXMRDKPOEW-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	2.0	0.0	142.89938762
4597	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/C11HN/c1-2-3-4-5-6-7-8-9-10-11-12/h1H	VSPOLSIHZRDJDD-UHFFFAOYSA-N	C11HN	147	0	molecule	HC11N	Cyanodecapentayne, Cyanopentaacetylene	VSPOLSIHZRDJDD-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	3.0	13.0	0.0	147.010899032

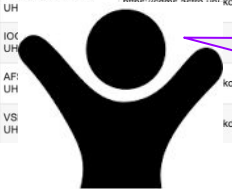
A deeper look to pyVAMDC

```
1 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max, species_df, nodes_df, verbose=True)
```

species_df
How to build it?

```
1 species_df , _ = species.getAllSpecies()
```

index	shortName	ivoIdentifier	inChI	inChIKey	stoichiometricFormula	massNumber	charge	speciesType	structuralFormula	name	did	tapEndpoint	lastIngestionScriptDate	speciesLastSeenOn	# unique atoms	# total atoms	computed charge	computed mol_weight
4584	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/C7HN/c1-2-3-4-5-6-7-8/h1H	XRJCSTPFBZTAPK-UHFFFAOYSA-N	C7HN	99	0	molecule	HCCCCCCCN	Cyanohexatriyne, Cyanotriacetylene	XRJCSTPFBZTAPK-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	3.0	9.0	0.0	99.010899032
4585	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/ClNO3/c1-5-2(3)4/i1+2	XYLGPCWDPLOBGP-NJFSPNSNSA-N	ClNO3	99	0	molecule	Cl-37-ONO2	Chlorine nitrate	XYLGPCWDPLOBGP-NJFSPNSNSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	3.0	5.0	0.0	98.95372045
4586	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/C7O/c1-2-3-4-5-6-7-8	ARYJKUMSSIOOOH-UHFFFAOYSA-N	C7O	100	0	molecule	C7O	Heptacarbon monoxide	ARYJKUMSSIOOOH-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	8.0	0.0	99.99491462
4587	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/Cl2O2/c1-3-4-2	MAYPHUUCLRDEAZ-UHFFFAOYSA-N	Cl2O2	Not provided	0	molecule	ClOOCl	Chlorine peroxide	MAYPHUUCLRDEAZ-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	4.0	0.0	101.9275346
4588	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/Cl2O2/c1-2-4-3	NKVCUZORVXMYQU-UHFFFAOYSA-N	Cl2O2	Not provided	0	molecule	ClClO2	Chloryl chloride	NKVCUZORVXMYQU-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	4.0	0.0	101.9275346
4589	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/Cl2O2/c1-3-4-2/i1+2	MAYPHUUCLRDEAZ-NJFSPNSNSA-N	Cl2O2	104	0	molecule	Cl-37-OOCl	Chlorine peroxide	MAYPHUUCLRDEAZ-NJFSPNSNSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	4.0	0.0	103.92458451
4590	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/BrO2/c2-1-3/i1-1	SISAYUDTHCIGLM-BJUDXGSMSA-N	BrO2	Not provided	0	molecule	OBr-79-O	Bromine dioxide	SISAYUDTHCIGLM-BJUDXGSMSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	3.0	0.0	110.90816634000001
4591	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/C8O/c1-2-3-4-5-6-7-8-9	XNKLVPGGOLSCFA-UHFFFAOYSA-N	C8O	112	0	molecule	C8O	Octacarbon monoxide	XNKLVPGGOLSCFA-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	9.0	0.0	111.99491462
4592	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/O2Se/c1-3-2/i3+1	JPJALAQPGMAKDF-LBPDFUHNSA-N	O2Se	112	0	molecule	Se-80-O2	Selenium dioxide	JPJALAQPGMAKDF-LBPDFUHNSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	3.0	0.0	111.90635054
4593	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/BrO2/c2-1-3/i1+1	SISAYUDTHCIGLM-OUBTZVSYSA-N	BrO2	113	0	molecule	OBr-81-O	Bromine dioxide	SISAYUDTHCIGLM-OUBTZVSYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	3.0	0.0	112.90611984
4594	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/C9O/c1-2-3-4-5-6-7-8-9-10	ZUGKIQCRTZHRDF-UHFFFAOYSA-N	C9O	124	0	molecule	C9O	Nonacarbon monoxide	ZUGKIQCRTZHRDF-UH	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	10.0	0.0	123.99491462
4595	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/S4/c1-3-4-2	IOOGPFMMGKCAGU-UHFFFAOYSA-N	S4	Not provided	0	molecule	S4	Tetrasulfur, Cyclo-tetrasulfur	IO(UH							
4596	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/IO/c1-2	AFSVSXMRDKPOEW-UHFFFAOYSA-N	IO	Not provided	0	molecule	IO	Iodine monoxide	AF UH	koeln.de/jpl/tap/	2025-					
4597	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/C11HN/c1-2-3-4-5-6-7-8-9-10-11-12/h1H	VSPOLSIHZRDJDD-UHFFFAOYSA-N	C11HN	147	0	molecule	HC11N	Cyanodecapentayne, Cyanopentaacetylene	VS UH	koeln.de/jpl/tap/	2025-					



And you can apply to this dataframe the custom filters!!!

A deeper look to pyVAMDC

```
1 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max, species_df, nodes_df, verbose=True)
```

species_df
How to build it?

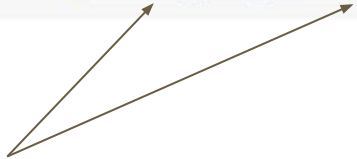
```
1 species_df , _ = species.getAllSpecies()
```

index	shortName	ivoIdentifier	inChI	inChIKey	stoichiometricFormula	massNumber	charge	speciesType	structuralFormula	name	did	tapEndpoint	lastIngestionScriptDate	speciesLastSeenOn	# unique atoms	# total atoms	computed charge	computed mol_weight
4584	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/C7HN/c1-2-3-4-5-6-7-8/h1H	XRJCSTPFBZTAPK-UHFFFAOYSA-N	C7HN	99	0	molecule	HCCCCCCCN	Cyanohexatriyne, Cyanotriacetylene	XRJCSTPFBZTAPK-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	3.0	9.0	0.0	99.010899032
4585	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/ClNO3/c1-5-2(3)4/i1+2	XYLGPCWDPLOBGP-NJFSPNSNSA-N	ClNO3	99	0	molecule	Cl-37-ONO2	Chlorine nitrate	XYLGPCWDPLOBGP-NJFSPNSNSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	3.0	5.0	0.0	98.95372045
4586	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/C7O/c1-2-3-4-5-6-7-8	ARYJKUMSSIOOOH-UHFFFAOYSA-N	C7O	100	0	molecule	C7O	Heptacarbon monoxide	ARYJKUMSSIOOOH-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	8.0	0.0	99.99491462
4587	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/Cl2O2/c1-3-4-2	MAYPHUUCLRDEAZ-UHFFFAOYSA-N	Cl2O2	Not provided	0	molecule	ClOOCl	Chlorine peroxide	MAYPHUUCLRDEAZ-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	4.0	0.0	101.9275346
4588	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/Cl2O2/c1-2-4-3	NKVCUZORVXMYQU-UHFFFAOYSA-N	Cl2O2	Not provided	0	molecule	ClClO2	Chloryl chloride	NKVCUZORVXMYQU-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	4.0	0.0	101.9275346
4589	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/Cl2O2/c1-3-4-2/i1+2	MAYPHUUCLRDEAZ-NJFSPNSNSA-N	Cl2O2	104	0	molecule	Cl-37-OOCl	Chlorine peroxide	MAYPHUUCLRDEAZ-NJFSPNSNSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	4.0	0.0	103.92458451
4590	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/BrO2/c2-1-3/i1-1	SISAYUDTHCIGLM-BJUDXGSMSA-N	BrO2	Not provided	0	molecule	OBr-79-O	Bromine dioxide	SISAYUDTHCIGLM-BJUDXGSMSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	3.0	0.0	110.90816634000001
4591	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/C8O/c1-2-3-4-5-6-7-8-9	XNKLVPGGOLSCFA-UHFFFAOYSA-N	C8O	112	0	molecule	C8O	Octacarbon monoxide	XNKLVPGGOLSCFA-UHFFFAOYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	9.0	0.0	111.99491462
4592	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/O2Se/c1-3-2/i3+1	JPJALAQPGMAKDF-LBPDFUHNSA-N	O2Se	112	0	molecule	Se-80-O2	Selenium dioxide	JPJALAQPGMAKDF-LBPDFUHNSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	3.0	0.0	111.90635054
4593	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/BrO2/c2-1-3/i1+1	SISAYUDTHCIGLM-OUBTZVSYSA-N	BrO2	113	0	molecule	OBr-81-O	Bromine dioxide	SISAYUDTHCIGLM-OUBTZVSYSA-N	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	3.0	0.0	112.90611984
4594	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/C9O/c1-2-3-4-5-6-7-8-9-10	ZUGKIQCRTZHRDF-UHFFFAOYSA-N	C9O	124	0	molecule	C9O	Nonacarbon monoxide	ZUGKIQCRTZHRDF-UH	https://cdms.astro.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	10.0	0.0	123.99491462
4595	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/S4/c1-3-4-2	IOOGPFMMGKCAGU-UHFFFAOYSA-N	S4	Not provided	0	molecule	S4	Tetrasulfur, Cyclo-tetrasulfur	IO(UH							
4596	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/IO/c1-2	AFSVSXMRDKPOEW-UHFFFAOYSA-N	IO	Not provided	0	molecule	IO	Iodine monoxide	AF UH	koeln.de/jpl/tap/	2025-					
4597	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc-tap_12.07	InChI=1S/C11HN/c1-2-3-4-5-6-7-8-9-10-11-12/h1H	VSPOLSIHZRDJDD-UHFFFAOYSA-N	C11HN	147	0	molecule	HC11N	Cyanodecapentayne, Cyanopentaacetylene	VS UH	koeln.de/jpl/tap/	2025-					

And you can apply to this dataframe the custom filters!!!

A deeper look to pyVAMDC

```
1 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max, species_df, nodes_df, verbose=True)
```



Thoses values must be in Angstrom

A deeper look to pyVAMDC

```
1 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max, species_df, nodes_df, verbose=True)
```

Thoses values must be in Angstrom

Energy Converters

```
import pyVAMDC.spectral.energyConverter as converter
```

A deeper look to pyVAMDC

```
1 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max, species_df, nodes_df, verbose=True)
```

Energy Converters

```
import pyVAMDC.spectral.energyConverter as converter
```

Converts from

- millijoule
- microjoule
- nanojoule
- picojoule
- eV
- erg
- kelvin
- rydberg
- cm-1
- hertz
- kilohertz
- megahertz
- gigahertz
- terahertz
- meter
- centimeter
- millimeter
- micrometer
- nanometer
- angstrom

To

- millijoule
- microjoule
- nanojoule
- picojoule
- eV
- erg
- kelvin
- rydberg
- cm-1
- hertz
- kilohertz
- megahertz
- gigahertz
- terahertz
- meter
- centimeter
- millimeter
- micrometer
- nanometer
- angstrom

A deeper look to pyVAMDC

```
1 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max, species_df, nodes_df, verbose=True)
```

Energy Converters

```
import pyVAMDC.spectral.energyConverter as converter
```

convert scalar values

```
converted_value = converter.electromagnetic_conversion(value_to_convert, from_unit="angstrom", to_unit="gigahertz")
```

convert columns

```
converted_df_column = converter.convert_dataframe_units(data_frame_to_convert, "ColumnToConvert", "angstrom", "ConvertedColumn", "gigahertz")
```

A deeper look to pyVAMDC

```
1 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max, species_df, nodes_df, verbose=True)
```

Energy Converters

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converted_df_column = converter.convert_dataframe_units(data_frame_to_convert, "ColumnToConvert", "angstrom", "ConvertedColumn", "gigahertz")
```

A deeper look to pyVAMDC

```
1 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max, species_df, nodes_df, verbose=True)
```

index	InchIKey	Inchl	Chemical name	Stoichiometric formula	Ordinary structural formula	Frequency	A	Lower energy(1/cm)	Lower total statistical weight	Lower nuclear statistical weight	Lower QNs	Upper energy(1/cm)	Upper total statistical weight	Upper nuclear statistical weight	Upper QNs	queryToken
13	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	161547004.713	0.0004614982856123	0.0	1	1.0	ElecStateLabel=X v=0 J=0	5388.628046	3	1.0	ElecStateLabel=X v=2 J=1	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
12	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	159935176.589	0.0013446262383399	27.857189	3	1.0	ElecStateLabel=X v=0 J=1	5362.720435	1	1.0	ElecStateLabel=X v=2 J=0	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
14	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	162264294.112	0.0005612928610076	27.857189	3	1.0	ElecStateLabel=X v=0 J=1	5440.411433	5	1.0	ElecStateLabel=X v=2 J=2	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
65	KEJOCWOXCDWNID-UHFFFAOYSA-N	1S/NO/c1-2/q+1	Nitrosylium, Nitrosyl ion	NO+	NO+	139684565.599	0.1954978883873505	0.0	3	NaN	ElecStateLabel=X v=0 J=0	4659.375574	9	NaN	ElecStateLabel=X v=2 J=1	cdms:8286be4e-6d60-4659-862d-7fd11f128228:get
11	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	159042585.919	0.0008802178686764	83.538419	5	1.0	ElecStateLabel=X v=0 J=2	5388.628046	3	1.0	ElecStateLabel=X v=2 J=1	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
15	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	162921269.08	0.0006088945785494	83.538419	5	1.0	ElecStateLabel=X v=0 J=2	5518.00699	7	1.0	ElecStateLabel=X v=2 J=3	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
10	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	158093572.368	0.000778623009123	166.977491	7	1.0	ElecStateLabel=X v=0 J=3	5440.411433	5	1.0	ElecStateLabel=X v=2 J=2	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
16	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	163517058.241	0.0006387816513122	166.977491	7	1.0	ElecStateLabel=X v=0 J=3	5621.319449	9	1.0	ElecStateLabel=X v=2 J=4	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
9	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	157089198.962	0.000727870791484	278.075338	9	1.0	ElecStateLabel=X v=0 J=4	5518.00699	7	1.0	ElecStateLabel=X v=2 J=3	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
17	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	164050831.663	0.000659817560053	278.075338	9	1.0	ElecStateLabel=X v=0 J=4	5750.222061	11	1.0	ElecStateLabel=X v=2 J=5	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
64	KEJOCWOXCDWNID-UHFFFAOYSA-N	1S/NO/c1-2/q+1	Nitrosylium, Nitrosyl ion	NO+	NO+	139448450.091	0.5835455216555205	3.975871	9	NaN	ElecStateLabel=X v=0 J=1	4655.475479	3	NaN	ElecStateLabel=X v=2 J=0	cdms:8286be4e-6d60-4659-862d-7fd11f128228:get
66	KEJOCWOXCDWNID-UHFFFAOYSA-N	1S/NO/c1-2/q+1	Nitrosylium, Nitrosyl ion	NO+	NO+	139799211.735	0.2351184976905347	3.975871	9	NaN	ElecStateLabel=X v=0 J=1	4667.175628	15	NaN	ElecStateLabel=X v=2 J=2	cdms:8286be4e-6d60-4659-862d-7fd11f128228:get
8	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	156030556.62	0.0006930428886986	416.700305	11	1.0	ElecStateLabel=X v=0 J=5	5621.319449	9	1.0	ElecStateLabel=X v=2 J=4	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
18	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	164521799.391	0.0006746629402928	416.700305	11	1.0	ElecStateLabel=X v=0 J=5	5904.55682	13	1.0	ElecStateLabel=X v=2 J=6	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
7	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	154918758.314	0.0006654469491119	582.688516	13	1.0	ElecStateLabel=X v=0 J=6	5750.222061	11	1.0	ElecStateLabel=X v=2 J=5	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
19	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	164929208.859	0.000688338404752	582.688516	13	1.0	ElecStateLabel=X v=0 J=6	6084.134749	15	1.0	ElecStateLabel=X v=2 J=7	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
6	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	153754932.243	0.0006431487976855	775.844335	15	1.0	ElecStateLabel=X v=0 J=7	5904.55682	13	1.0	ElecStateLabel=X v=2 J=6	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
20	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	165272341.18	0.0006975063069331	775.844335	15	1.0	ElecStateLabel=X v=0 J=7	6288.736229	17	1.0	ElecStateLabel=X v=2 J=8	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
63	KEJOCWOXCDWNID-UHFFFAOYSA-N	1S/NO/c1-2/q+1	Nitrosylium, Nitrosyl ion	NO+	NO+	139326988.819	0.3879340831149696	11.927478	15	NaN	ElecStateLabel=X v=0 J=2	4659.375574	9	NaN	ElecStateLabel=X v=2 J=1	cdms:8286be4e-6d60-4659-862d-7fd11f128228:get

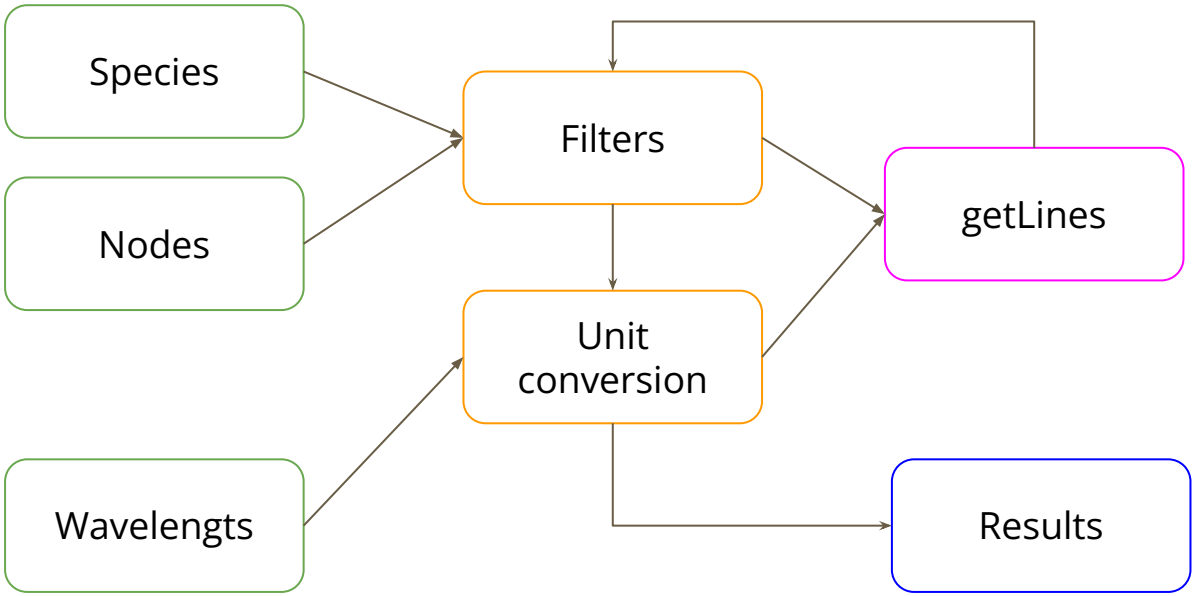
A deeper look to pyVAMDC

```
1 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max, species_df, nodes_df, verbose=True)
```

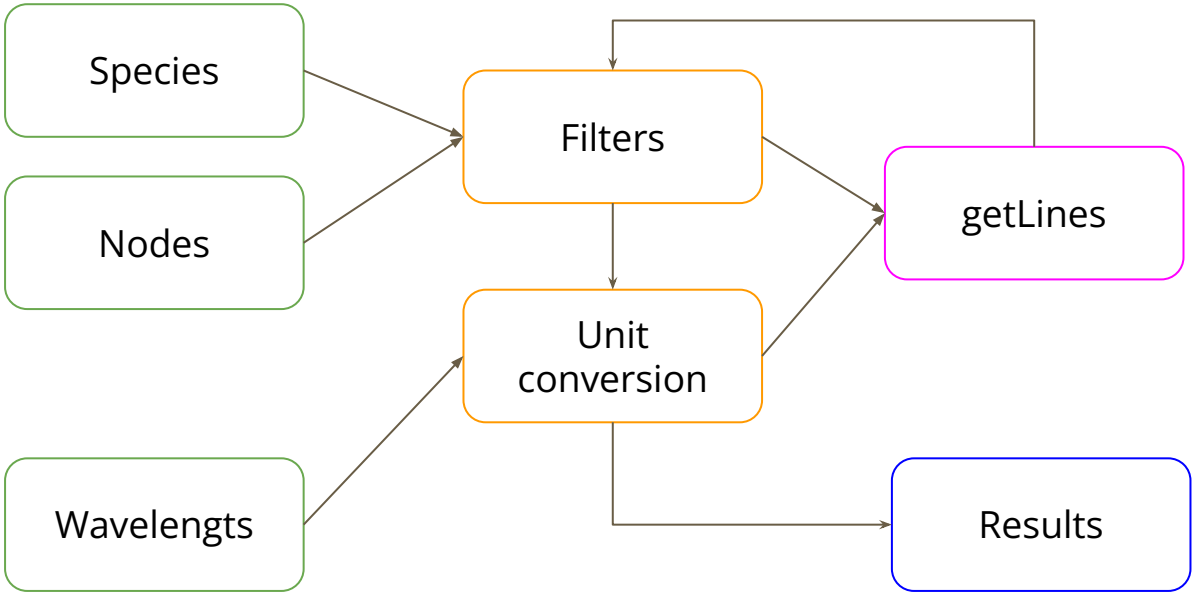
index	InchIKey	Inchl	Chemical name	Stoichiometric formula	Ordinary structural formula	Frequency	A	Lower energy(1/cm)	Lower total statistical weight	Lower nuclear statistical weight	Lower QNs	Upper energy(1/cm)	Upper total statistical weight	Upper nuclear statistical weight	Upper QNs	queryToken
13	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	161547004.713	0.0004614982856123	0.0	1	1.0	ElecStateLabel=X v=0 J=0	5388.628046	3	1.0	ElecStateLabel=X v=2 J=1	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
12	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	159935176.589	0.0013446262383399	27.857189	3	1.0	ElecStateLabel=X v=0 J=1	5362.720435	1	1.0	ElecStateLabel=X v=2 J=0	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
14	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	162264294.112	0.0005612928610076	27.857189	3	1.0	ElecStateLabel=X v=0 J=1	5440.411433	5	1.0	ElecStateLabel=X v=2 J=2	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
65	KEJOCWOXCDWNID-UHFFFAOYSA-N	1S/NO/c1-2/q+1	Nitrosylium, Nitrosyl ion	NO+	NO+	139684565.599	0.1954978883873505	0.0	3	NaN	ElecStateLabel=X v=0 J=0	4659.375574	9	NaN	ElecStateLabel=X v=2 J=1	cdms:8286be4e-6d60-4659-862d-7fd11f128228:get
11	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	159042585.919	0.0008802178686764	83.538419	5	1.0	ElecStateLabel=X v=0 J=2	5388.628046	3	1.0	ElecStateLabel=X v=2 J=1	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
15	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	162921269.08	0.0006088945785494	83.538419	5	1.0	ElecStateLabel=X v=0 J=2	5518.00699	7	1.0	ElecStateLabel=X v=2 J=3	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
10	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	158093572.368	0.000778623009123	166.977491	7	1.0	ElecStateLabel=X v=0 J=3	5440.411433	5	1.0	ElecStateLabel=X v=2 J=2	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
16	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	163517058.241	0.0006387816513122	166.977491	7	1.0	ElecStateLabel=X v=0 J=3	5621.319449	9	1.0	ElecStateLabel=X v=2 J=4	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
9	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	157089198.962	0.000727870791484	278.075338	9	1.0	ElecStateLabel=X v=0 J=4	5518.00699	7	1.0	ElecStateLabel=X v=2 J=3	cdms:a384a34a-4739-4aa2-ae54-c63ee4882c8d:get
17	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	164050831.663	0.000659817560053	278.075338	9	1.0	ElecStateLabel=X v=0 J=4					
64	KEJOCWOXCDWNID-UHFFFAOYSA-N	1S/NO/c1-2/q+1	Nitrosylium, Nitrosyl ion	NO+	NO+	139448450.091	0.5835455216555205	3.975871	9	NaN	ElecStateLabel=X v=0 J=1					
66	KEJOCWOXCDWNID-UHFFFAOYSA-N	1S/NO/c1-2/q+1	Nitrosylium, Nitrosyl ion	NO+	NO+	139799211.735	0.2351184976905347	3.975871	9	NaN	ElecStateLabel=X v=0 J=1					
8	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	156030556.62	0.0006930428886986	416.700305	11	1.0	ElecStateLabel=X v=0 J=5					
18	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	164521799.391	0.0006746629402928	416.700305	11	1.0	ElecStateLabel=X v=0 J=5					
7	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	154918758.314	0.0006654469491119	582.688516	13	1.0	ElecStateLabel=X v=0 J=6					
19	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	164929208.859	0.000688338404752	582.688516	1							
6	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	153754932.243	0.0006431487976855	775.844335	1		StateLab J=7					
20	WVVLBIYUCXYYEU-UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	165272341.18	0.0006975063069331	775.844335	1		StateLabel=X J=7					
63	KEJOCWOXCDWNID-UHFFFAOYSA-N	1S/NO/c1-2/q+1	Nitrosylium, Nitrosyl ion	NO+	NO+	139326988.819	0.3879340831149696	11.927478	1		StateLabel=X J=2	4659				7fd11f128228:get

- All the data are fetched - no coutout!!
- You can apply to this dataframe the custom filters and column unit conversions!!!

Wrapping up


Species
Nodes
Wavelengts
Filters
Unit conversion
getLines
Results

Wrapping up



Consider the scenario :

By extracting data from CDMS and Hitran, get all the spectroscopic information in the wavelenght range between 1 and 3 micrometer, for all the molecules composed of 1 to 4 atoms, containing C, H, N, O, S and not containing Ca, Li, He, Na, Mg. In the result convert the energies from cm^-1 to Kelvin and take only the Lower Energy level where the quantum numbers v is equal to 0.

→ **That's only a few lines of pyVAMDC.**

Conclusion and further works

- We are working on new functionalities
  - getSpeciedByAstrophysicalDomain
  - getLinesByTelescopeBand (ex. AlmaBands from 1 to 10)

- We are trying to fetch data faster
  - interoperability is a series of adapters and wrappers → slow down data retrieval.
    - Good ratio between parallel tasks and saturation of the ressources?

- We are developing new modules for collisional processes
  - getRadex(target, collider)

- Building functionalities directly on users' needs.