





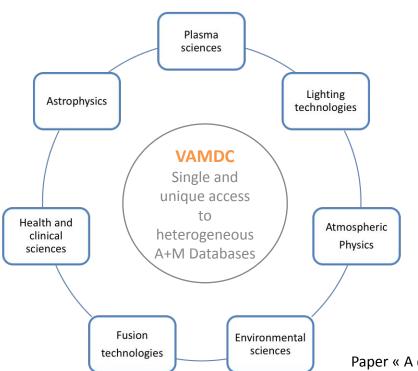
The pyVAMDC library

Interop-2025@CollegePark





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

VAMDC is nice, but...

Too complex to use! Steep learning curve!



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```
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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Too complex to use! Steep learning curve!





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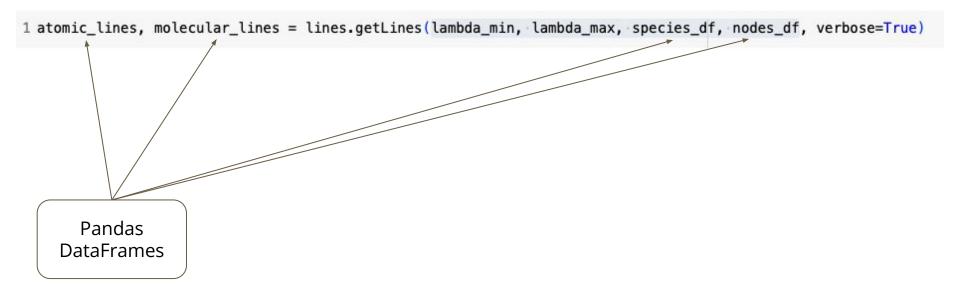
https://github.com/VAMDC/pyVAMDC/

That's it. Thank you for your attention...

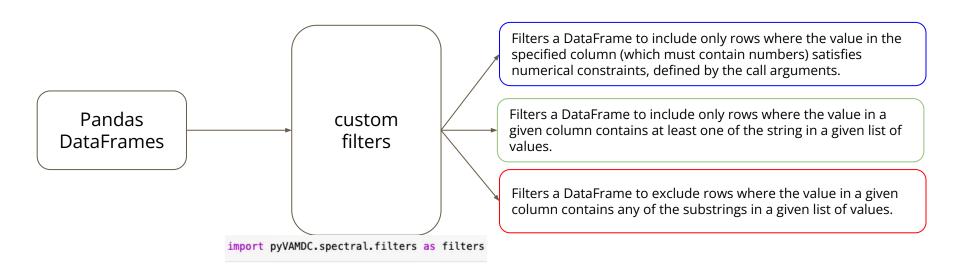
```
1 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max, species_df, nodes_df, verbose=True)
```

```
Optional fields

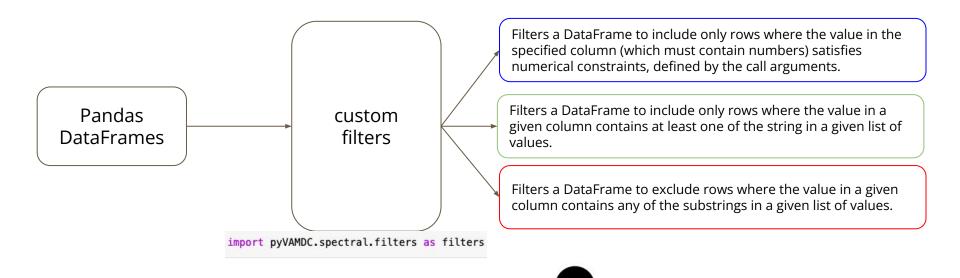
1 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max, species_df, nodes_df, verbose=True)
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1 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max, species_df, nodes_df, verbose=True)



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



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

```
1 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max, species_df, nodes_df, verbose=True)
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nodes_df How to build it?

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

nodes_df How to build it?

1 nodes_df = species.getNodeHavingSpecies()
2 nodes df

									1 to 25 of 32 entries Filter
index	shortName A	description	contactEmail	ivoldentifier	tapEndpoint	referenceUrl	lastUpdate	lastSeen	topics
1 A	Col - database for collisional processes		vlada@ipb.ac.rs	ivo://vamdc/acol	http://servo.aob.rs/acol/tap/	http://servo.aob.rs/acol	2025-02-12 15:47:44	2025-02- 12 2025-02-12	Atomic states,Atoms,Collisions,Molecular states,Molecules
2 A	MDIS 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 A	cetylene Spectroscopic Databank 1000K (VAMDC- AP)		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 B	ASECOL2015: 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
4 B	elgrade electron/atom(molecule) database (BEAMDB)		bratislav.marinkovic@ipb.ac.rs	ivo://vamdc/emol_radam	http://servo.aob.rs/emol/tap/	http://servo.aob.rs/emol/	2025-02-12 15:47:44	2025-02- 12 2025-02-12	Atomic states, Atoms, Collisions, Molecular states, Molecules
8 C	DMS		endres@ph1.uni-koeln.de	ivo://vamdc/cdms/vamdc- tap_12.07	https://cdms.astro.uni-koeln.de/cdms/tap/	https://cdms.astro.uni-koeln.de	2025-02-12 15:47:44	2025-02- 12 2025-02-12	Atomic states, Atoms, Molecular states, Molecules, Radiative transitions
	arbon Dioxide Spectroscopic Databank 1000K /AMDC-TAP)		vip@lts.iao.ru	ivo://vamdc/cdsd-1000	http://lts.iao.ru/node/cdsd-1000-xsams1/tap/	ftp://ftp.iao.ru/pub/CDSD-1000/	2025-02-12 15:47:44	2025-02- 12 2025-02-12	Molecular states, Molecules, Radiative transitions, Radiative transitions shifting
	arbon Dioxide Spectroscopic Databank 296K /AMDC-TAP)		vip@lts.iao.ru	ivo://vamdc/cdsd-296	http://lts.iao.ru/node/cdsd-296-xsams1/tap/	ftp://ftp.iao.ru/pub/CDSD-1000/	2025-02-12 15:47:44	2025-02- 12 2025-02-12	Molecular states, Molecules, Radiative transitions, Radiative transitions shifting
	arbon Dioxide Spectroscopic Databank 4000K /AMDC-TAP)		vip@lts.iao.ru	ivo://vamdc/cdsd-4000	http://lts.iao.ru/node/cdsd-4000-xsams1/tap/	ftp://ftp.iao.ru/pub/CDSD-4000/	2025-02-12 15:47:44	2025-02- 12 2025-02-12	Molecular states, Molecules, Radiative transitions, Radiative transitions shifting
9 C	hianti		gtr@ast.cam.ac.uk	ivo://vamdc/chianti/django		http://www.chianti.rl.ac.uk/	2025-02-12 15:47:44	2025-02- 12 2025-02-12	Atomic states,Atoms,Radiative transitions
	eCaSDa: Gemane Calculated Spectroscopic latabase		cyril.richard@u-bourgogne.fr	ivo://vamdc/dijon-GeH4-lines	http://vamdc.icb.cnrs.fr/gecasda/tap/	http://vamdc.icb.cnrs.fr/PHP/gecasda.php	2025-02-12 15:47:44	2025-02- 12 2024-07-22	Molecular states, Molecules, Radiative transitions
11 H	itran (VAMDC-TAP)		Ch.Hill@iaea.org	ivo://vamdc/hitran/vamdc- working	https://hitran.org/tap/		2025-02-12 15:47:44	2025-02-12 2025-02-12	Molecular states, Molecules, Radiative transitions

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

nodes_df How to build it?

1 nodes_df = species.getNodeHavingSpecies()
2 nodes_df

									1 10 20 01 02 0111100 (11111
index	shortName A	description	contactEmail	ivoldentifier	tapEndpoint	referenceUrl	lastUpdate	lastSeen	topics
1 ACo	I - database for collisional processes		vlada@ipb.ac.rs	ivo://vamdc/acol	http://servo.aob.rs/acol/tap/	http://servo.aob.rs/acol	2025-02-12 15:47:44	2025-02- 12 2025-02-12	Atomic states, Atoms, Collisions, Molecular states, Molecules
2 AME	DIS 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
o Acet	tylene Spectroscopic Databank 1000K (VAMDC-		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 BAS	ECOL2015: 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
4 Belg	rade electron/atom(molecule) database (BEAMDB)		bratislav.marinkovic@ipb.ac.rs	ivo://vamdc/emol_radam	http://servo.aob.rs/emol/tap/	http://servo.aob.rs/emol/	2025-02-12 15:47:44	2025-02- 12 2025-02-12	Atomic states, Atoms, Collisions, Molecular states, Molecules
8 CDM	MS		endres@ph1.uni-koeln.de	ivo://vamdc/cdms/vamdc- tap_12.07	https://cdms.astro.uni-koeln.de/cdms/tap/	https://cdms.astro.uni-koeln.de	2025-02-12 15:47:44	2025-02- 12 2025-02-12	Atomic states, Atoms, Molecular states, Molecules, Radiative transitions
	oon Dioxide Spectroscopic Databank 1000K MDC-TAP)		vip@lts.iao.ru	ivo://vamdc/cdsd-1000	http://lts.iao.ru/node/cdsd-1000-xsams1/tap/	ftp://ftp.iao.ru/pub/CDSD-1000/	2025-02-12 15:47:44	2025-02- 12 2025-02-12	Molecular states, Molecules, Radiative transitions, Radiative transitions shifting
6 Carb	oon Dioxide Spectroscopic Databank 296K MDC-TAP)		vip@lts.iao.ru	ivo://vamdc/cdsd-296	http://lts.iao.ru/node/cdsd-296-xsams1/tap/	ftp://ftp.iao.ru/pub/CDSD-1000/	2025-02-12 15:47:44	2025-02- 12 2025-02-12	Molecular states, Molecules, Radiative transitions, Radiative transitions shifting
7 Carb (VAN	oon Dioxide Spectroscopic Databank 4000K MDC-TAP)		vip@lts.iao.ru	ivo://vamdc/cdsd-4000	http://lts.iao.ru/node/cdsd-4000-xsams1/tap/	ftp://ftp.iao.ru/pub/CDSD-4000/	2025-02-12 15:47:44	2025-02- 12 2025-02-12	Molecular states, Molecules, Radiative transitions, Radiative transitions shifting
9 Chia	nnti		gtr@ast.cam.ac.uk	ivo://vamdc/chianti/django		A	2025		1
	aSDa: Gemane Calculated Spectroscopic abase		cyril.richard@u-bourgogne.fr	ivo://vamdc/dijon-GeH4-lines	http://vamdc.icb.cnrs.fr/gecasda/tap	HP/geo.	$\overline{}$	_	ou can apply to this
11 Hitra	an (VAMDC-TAP)		Ch.Hill@iaea.org	ivo://vamdc/hitran/vamdc- working	https://hitran.org/tap/		2	data	frame the custom
									filters!!!

1 to 25 of 32 entries Filter L

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ndex	shortName 🛦	description	contactEmail	ivoldentifier	tapEndpoint	referenceUrl	lastUpdate	lastSeen	topics
1	ACol - database for collisional processes		vlada@ipb.ac.rs	ivo://vamdc/acol	http://servo.aob.rs/acol/tap/	http://servo.aob.rs/acol	2025-02-12 15:47:44	2025-02- 12 2025-02-12	Atomic states,Atoms,Collisions,Molecular states,Molecules
	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
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	Carbon Dioxide Spectroscopic Databank 4000K (VAMDC-TAP)		vip@lts.iao.ru	ivo://vamdc/cdsd-4000	http://lts.iao.ru/node/cdsd-4000-xsams1/tap/	ftp://ftp.iao.ru/pub/CDSD-4000/	2025-02-12 15:47:44	2025-02- 12 2025-02-12	Molecular states, Molecules, Radiative transitions, Radiative transitions shifting
9	Chianti		gtr@ast.cam.ac.uk	ivo://vamdc/chianti/django		ď	2025		
10	GeCaSDa: Gemane Calculated Spectroscopic Database		cyril.richard@u-bourgogne.fr	ivo://vamdc/dijon-GeH4-lines	http://vamdc.icb.cnrs.fr/gecasda/tap	HP/geo.		\nd yc	ou can apply to this
11	Hitran (VAMDC-TAP)		Ch.Hill@iaea.org	ivo://vamdc/hitran/vamdc- working	https://hitran.org/tap/		2	datat	frame the custom

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1 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max, species_df, nodes_df, verbose=True)
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species_df How to build it?

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index	shortName	ivoldentifier	InChi	InChiKey	stoichiometricFormula	massNumber .	charge speciesType	structuralFormula	a name	did	tapEndpoint	lastingestionScriptDate	speciesLastSeenOn	# unique atoms	# total atoms	computed charge	computed mol_weight
4584 V	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc- tap_12.07		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 V	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc- tap_12.07	InChI=1S/CINO3/c1-5- 2(3)4/I1+2	XYLGPCWDPLOBGP- NJFSPNSNSA-N	CINO3	99	0 molecule	CI-37-ONO2		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 V	JPL database: VAMDC-TAP service			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 V	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc- tap_12.07	InChI=1S/Cl2O2/c1-3-4-2	MAYPHUUCLRDEAZ- UHFFFAOYSA-N	CI2O2	Not provided	0 molecule	CIOOCI		MAYPHUUCLRDEAZ- UHFFFAOYSA-N	https://cdms.astro.uni-koein.de/jpl/tap/	2025-02-12	2025-02-12	2.0	4.0	0.0	101.9275346
4588 V	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc- tap_12.07	InChl=1S/Ci2O2/c1-2-4-3	NKVCUZORVXMYQU- UHFFFAOYSA-N	CI2O2	Not provided	0 molecule	CICIO2		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 V	JPL database: VAMDC-TAP service		InChl=1S/Cl2O2/c1-3-4- 2/i1+2	MAYPHUUCLRDEAZ- NJFSPNSNSA-N	CI2O2	104	0 molecule	CI-37-OOCI		MAYPHUUCLRDEAZ- NJFSPNSNSA-N	https://cdms.astro.uni-koein.de/jpl/tap/	2025-02-12	2025-02-12	2.0	4.0	0.0	103.92458451
4590 V	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc- tap_12.07	InChl=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 V	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 V	JPL database: VAMDC-TAP service		InChl=1S/O2Se/c1-3- 2/i3+1	JPJALAQPGMAKDF- LBPDFUHNSA-N	O2Se	112	0 molecule	Se-80-O2		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 V	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc- tap_12.07	InChl=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 V	JPL database: VAMDC-TAP service		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 V	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc- tap_12.07	InChl=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 V	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc- tap_12.07	InChI=1S/IO/c1-2	AFSVSXMRDKPOEW- UHFFFAOYSA-N	Ю	Not provided	0 molecule	Ю	lodine 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 V	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc- tap_12.07	InChl=1S/C11HN/c1-2-3-4- 5-6-7-8-9-10-11-12/h1H	VSPOLSIHZRDJDD- UHFFFAOYSA-N	C11HN	147	0 molecule	HC11N		VSPOLSIHZRDJDD- UHFFFAOYSA-N	https://cdms.astro.uni-koein.de/jpl/tap/	2025-02-12	2025-02-12	3.0	13.0	0.0	147.010899032

InChi=1S/C11HN/c1-2-3-4- VSPOLSIHZRDJDD-

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()

ivo://vamdc/ipl/vamdc-

4597 VAMDC-TAP

index	shortName	ivoldentifier	InChi	InChlKey	stoichiometricFormula	massNumber c	harge speciesType	structuralFormula	a name	did	tapEndpoint	lastIngestionScriptDat.	te speciesLastSeenOn	# unique atoms	# total atoms	computed charge	computed mol_weigh
4584 V	JPL database: VAMDC-TAP service		InChI=1S/C7HN/c1-2-3-4- 5-6-7-8/h1H	XRJCSTPFBZTAPK- UHFFFAOYSA-N	C7HN	99	0 molecule	HCCCCCCCN		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		InChl=1S/CINO3/c1-5- 2(3)4/l1+2	XYLGPCWDPLOBGP- NJFSPNSNSA-N	CINO3	99	0 molecule	CI-37-ONO2		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 V	JPL database: VAMDC-TAP service		InChl=1S/C7O/c1-2-3-4-5- 6-7-8	ARYJKUMSSIOOOH- UHFFFAOYSA-N	C70	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 V	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc- tap_12.07	InChl=1S/Cl2O2/c1-3-4-2	MAYPHUUCLRDEAZ- UHFFFAOYSA-N	CI2O2	Not provided	0 molecule	CIOOCI		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 V	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc- tap_12.07	InChl=1S/Cl2O2/c1-2-4-3	NKVCUZORVXMYQU- UHFFFAOYSA-N	CI2O2	Not provided	0 molecule	CICIO2		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		InChl=1S/Cl2O2/c1-3-4- 2/i1+2	MAYPHUUCLRDEAZ- NJFSPNSNSA-N	CI2O2	104	0 molecule	CI-37-OOCI		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 V	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc- tap_12.07	InChl=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 V	JPL database: VAMDC-TAP service			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 V	JPL database: VAMDC-TAP service		InChl=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 V	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc- tap_12.07	InChl=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 V	JPL database: VAMDC-TAP service		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://odms.netm.uni-koeln.de/jpl/tap/	2025-02-12	2025-02-12	2.0	10.0	0.0	123.99491462
4595 V	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc- tap_12.07	InChl=1S/S4/c1-3-4-2	IOOGPFMMGKCAGU- UHFFFAOYSA-N	S4	Not provided	0 molecule	S4	Tetrasulfur, Cyclo- tetrasulfur	IOC		A	nd you	can.	app	v to the	his)
4596 V	JPL database: VAMDC-TAP service	ivo://vamdc/jpl/vamdc- tap_12.07	InChi=1S/IO/c1-2	AFSVSXMRDKPOEW- UHFFFAOYSA-N	Ю	Not provided	0 molecule	Ю	lodine monoxide	AF: UH	koeln.de/jpl/tap/		datafra				
	IPI datahase:												AACATT (• •

Cyanodecapentayne.

Cvanopentaacetylene

koeln.de/jpl/tap/ 2025-

filters!!!

HC11N

IOOGPFMMGKCAGU-

AFSVSXMRDKPOEW-

UHFFFAOYSA-N

UHFFFAOYSA-N

UHFFFAOYSA-N

InChl=1S/C11HN/c1-2-3-4- VSPOLSIHZRDJDD

Not provided

Not provided

147

1 species_df , _ = species.getAllSpecies()

JPL database

JPL database

4595 VAMDC-TAP

4596 VAMDC-TAP

service

4597 VAMDC-TAP

service

ivo://vamdc/jpl/vamdc-

ivo://vamdc/ipl/vamdc-

tap 12.07

tap 12.07

InChl=1S/S4/c1-3-4-2

InChl=1S/IO/c1-2

5-6-7-8-9-10-11-12/h1H

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

species_df
How to build it?

shortName ivoldentifier InChi InChlKev stoichiometricFormula massNumber charge speciesType structuralFormula tanEndnoint lastingestionScriptDate species astSeenOn # unique atoms # total atoms computed charge computed mol weight JPL database InChl=1S/C7HN/c1-2-3-4-XRJCSTPFBZTAPK-XRJCSTPFBZTAPK ivo://vamdc/ipl/vamdc-Cvanohexatrivne 4584 VAMDC-TAP HCCCCCCCN https://cdms.astro.uni-koeln.de/ipl/tap/ 2025-02-12 3.0 99.010899032 tap_12.07 5-6-7-8/h1H UHFFFAOYSA-N Cyanotriacetylene UHFFFAOYSA-N service JPL database ivo://vamdc/jpl/vamdc-InChI=1S/CINO3/c1-5-XYLGPCWDPLOBGP-XYLGPCWDPLOBGP CINO3 4585 VAMDC-TAP 99 CI-37-ONO2 Chlorine nitrate https://cdms.astro.uni-koeln.de/jpl/tap/ 2025-02-12 2025-02-12 3.0 5.0 0.0 98.95372045 tap 12.07 NJFSPNSNSA-N NJFSPNSNSA-N service JPI database ivo://vamdc/jpl/vamdc-InChl=1S/C7O/c1-2-3-4-5-ARYJKUMSSIOOOH-ARYJKUMSSIOOOH-C70 4586 VAMDC-TAP 100 Heptacarbon monoxide https://cdms.astro.uni-koeln.de/ipl/tap/ 2025-02-12 2025-02-12 2.0 8.0 0.0 99.99491462 UHFFFAOYSA-N UHEFFAOYSA-N tap_12.07 service JPL database ivo://vamdc/inl/vamdc MAYPHULICI RDEAZ MAYPHUUCLRDEAZ-4587 VAMDC-TAP InChl=1S/Cl2O2/c1-3-4-2 CI2O2 Not provided 0 molecule CIOOCI Chlorine peroxide https://cdms.astro.uni-koeln.de/ipl/tap/ 2025-02-12 2025-02-12 2.0 4.0 0.0 UHFFFAOYSA-N tap_12.07 UHFFFAOYSA-N convice JPL database ivo://vamdc/jpl/vamdo NKVCUZORVXMYQU-**NKVCUZORVXMYQU** InChl=1S/Cl2O2/c1-2-4-3 CICIO2 https://cdms.astro.uni-koeln.de/ipl/tap/ 2025-02-12 2.0 4.0 0.0 101.9275346 4588 VAMDC-TAP Not provided Chloryl chloride UHFFFAOYSA-N 0 molecule UHFFFAOYSA-N tap 12.07 JPL database InChl=1S/Cl2O2/c1-3-4-MAYPHUUCLRDEAZ-MAYPHUUCLRDEAZ-4589 VAMDC-TAP CI2O2 104 CI-37-OOCI Chlorine peroxide https://cdms.astro.uni-koeln.de/jpl/tap/ 2025-02-12 2.0 4.0 0.0 103.92458451 tap_12.07 NJFSPNSNSA-N NJFSPNSNSA-N service .IPI database SISAYUDTHCIGLM-SISAYUDTHCIGLMivo://vamdc/ipl/vamdc-4590 VAMDC-TAP InChl=1S/BrO2/c2-1-3/i1-BrO2 Not provided OBr-79-O Bromine dioxide https://cdms.astro.uni-koeln.de/jpl/tap/ 2025-02-12 2025-02-12 2.0 3.0 0.0 110.90816634000001 B.IUDYGSMSA.N BJUDXGSMSA-N tap_12.07 service JPL database InChl=1S/C8O/c1-2-3-4-5-XNKI VPGGOI SCEA. YNKI VPGGOLSCEA. ivo-//vamdc/inl/vamdc-VAMDC-TAP C80 112 Octacarbon monoxide https://cdms.astro.uni-koeln.de/ipl/tap/ 2025-02-12 2025-02-12 2.0 9.0 0.0 111.99491462 0 molecule tap_12.07 UHFFFAOYSA-N UHFFFAOYSA-N JPL database ivo://vamdc/jpl/vamdc-**JPJALAQPGMAKDF JPJALAQPGMAKDF** 4592 VAMDC-TAP O2Se 112 0 molecule Se-80-O2 Selenium dioxide https://cdms.astro.uni-koeln.de/jpl/tap/ 2025-02-12 2025-02-12 2.0 3.0 0.0 111.90635054 tap 12.07 LBPDFUHNSA-N LBPDFUHNSA-N JPI database ivo://vamdc/ipl/vamdc-SISAYUDTHCIGLM-SISAYUDTHCIGLM-4593 VAMDC-TAP InChl=1S/BrO2/c2-1-3/i1+1 BrO2 113 0 molecule OBr-81-O Bromine dioxide https://cdms.astro.uni-koeln.de/ipl/tap/ 2025-02-12 2025-02-12 2.0 3.0 0.0 112.90611984 tap_12.07 OUBTZVSYSA-N service IPI database InChl=1S/C9O/c1-2-3-4-5-ZUGKIQCRTZHRDF ZUGKIQCRTZHRDF ivo://vamdc/ipl/vamdc-4594 VAMDC-TAP C90 124 C90 Nonacarbon monoxide https://odms.actro.uni-koeln.de/jpl/tap/ 2025-02-12 2025-02-12 2.0 0.0 123.99491462 tap_12.07 6-7-8-9-10 UHFFFAOYSA-N service

Tetrasulfur, Cyclo-

lodine monoxide

Cyanodecapentayne.

Cvanopentaacetylene

UH

VS

tetrasulfur

HC11N

And you can apply to this

dataframe the custom

filters!!!

koeln.de/jpl/tap/ 2025-

koeln.de/jpl/tap/ 2025-

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

Thoses values must be in Angstrom

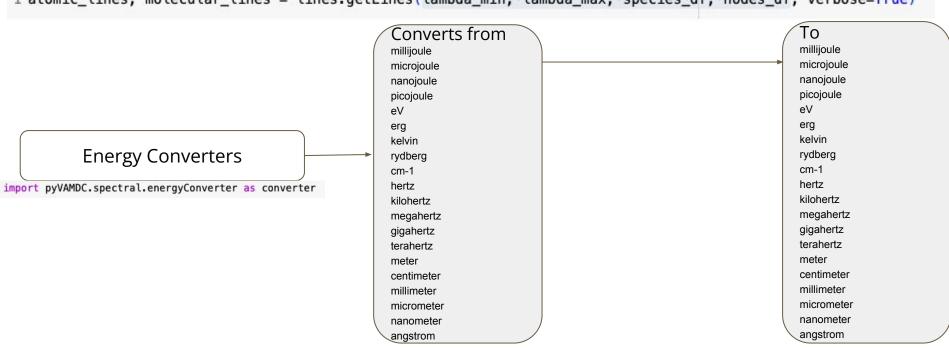
```
1 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max, species_df, nodes_df, verbose=True)
```

Thoses values must be in Angstrom

Energy Converters

import pyVAMDC.spectral.energyConverter as converter

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



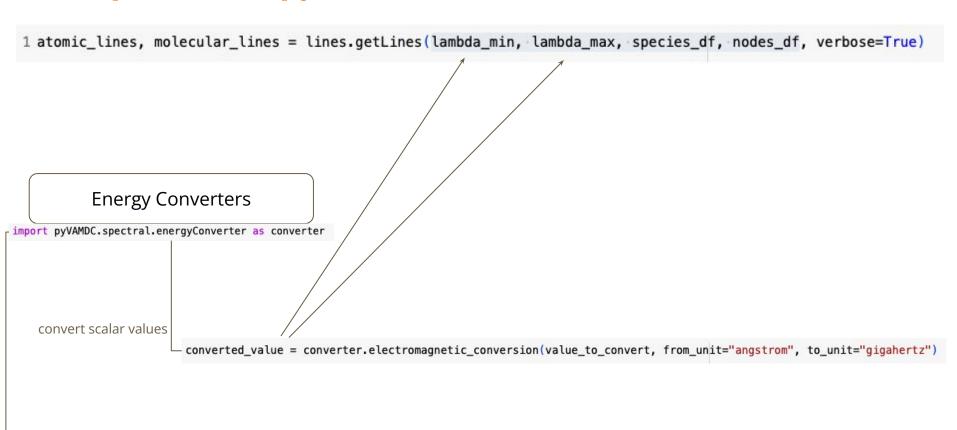
convert columns

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



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

convert columns



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

CH+

CH+

CH+

NO+

NO+

CH+

CH+

CH+

CH+

CH+

CH+

NO+

163517058.241 0.0006387816513122

157089198.962 0.000727870791484

164050831.663 0.000659817560053

139448450.091 0.5835455216555205

139799211.735 0.2351184976905347

156030556.62 0.0006930428886986

164521799.391 0.0006746629402928

154918758.314 0.0006654469491119

164929208.859 0.000688338404752

153754932.243 0.0006431487976855

165272341.18 0.0006975063069331

139326988.819 0.3879340831149696

WVVLBIYUCXYYEU-16 UHFFFAOYSA-N

WVVLBIYUCXYYEU-9 UHFFFAOYSA-N

17 WVVLBIYUCXYYEU-UHFFFAOYSA-N

UHFFFAOYSA-N

WVVLBIYUCXYYEU-8 UHFFFAOYSA-N

WVVLBIYUCXYYEU-18 UHFFFAOYSA-N

WVVLBIYUCXYYEU-

UHFFFAOYSA-N

19 WVVLBIYUCXYYEU-UHFFFAOYSA-N

WVVLBIYUCXYYEU-6 UHFFFAOYSA-N

WVVLBIYUCXYYEU-

KEJOCWOXCDWNID- 1S/NO/c1-

UHFFFAOYSA-N

UHFFFAOYSA-N

66 UHFFFAOYSA-N

KEJOCWOXCDWNID- 1S/NO/c1-

KEJOCWOXCDWNID- 1S/NO/c1-

1S/CH/h1H/q+1 Methylidynium CH+

1S/CH/h1H/q+1 Methylidynium CH+

1S/CH/h1H/g+1 Methylidynium CH+

Nitrosylium,

Nitrosyl ion

Nitrosylium,

Nitrosyl ion

1S/CH/h1H/q+1 Methylidynium

1S/CH/h1H/q+1 Methylidynium CH+

Nitrosylium.

NO+

NO+

	1 atomi	.c_lir	nes, m	olecula	r_lines =	line	es.getL	ines(la	mbda_min,	lambda_ma	x, spe	cies_d	f, nodes_	df, verbos	e=Tru	e)
		4														
index	InchlKey WVVLBIYUCXYYEU- UHFFFAOYSA-N	Inchl 1S/CH/h1H/q+1	Methylidynium	CH+	Ordinary structural formula		0.0004614982856123		Lower total statistical weight	Lower nuclear statistical weight	Lower QNs ElecStateLabel=X v=0 J=0		Upper total statistical weight	Upper nuclear statistical weight	ElecStatel abol=Y	queryToken cdms:a384a34a 4739-4aa2-ae54 c63ee4882c8d:g
12	WVVLBIYUCXYYEU- UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	159935176.589	0.0013446262383399	27.857189	3	3 1.0	ElecStateLabel=X v=0 J=1	5362.720435	1	1.0	ElecStateLabel=X v=2 J=0	
14	WVVLBIYUCXYYEU- UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	162264294.112	0.0005612928610076	27.857189	3	3 1.0	ElecStateLabel=X v=0 J=1	5440.411433		1.0	ElecStateLabel=X v=2 J=2	cdms:a384a34a- 4739-4aa2-ae54 c63ee4882c8d:g
65	KEJOCWOXCDWNID- UHFFFAOYSA-N	1S/NO/c1- 2/q+1	Nitrosylium, Nitrosyl ion	NO+	NO+	139684565.599	0.1954978883873505	0.0	3	3 NaN	ElecStateLabel=X v=0 J=0	4659.375574	5	NaN	ElecStateLabel=X v=2 J=1	cdms:8286be4e- 6d60-4659-862d 7fd11f128228:ge
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:g
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:g
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		1.0	ElecStateLabel=X v=2 J=2	cdms:a384a34a- 4739-4aa2-ae54 c63ee4882c8d:g

11

11

13

13

15

15

15

166.977491

278.075338

278.075338

3,975871

3.975871

416.700305

416.700305

582.688516

582.688516

775.844335

775.844335

11.927478

1.0 ElecStateLabel=X

1.0 ElecStateLabel=X

1.0 ElecStateLabel=X

ElecStateLabel=X

v=0 J=3

v=0 J=4

v=0 J=4

v=0 J=1

v=0 J=1

v=0 J=5

v=0 J=5

v=0 J=6

NaN ElecStateLabel=X

1.0 ElecStateLabel=X

1.0 ElecStateLabel=X

1.0 ElecStateLabel=X

1.0 ElecStateLabel=X v=0 J=6

1.0 ElecStateLabel=X

1.0 ElecStateLabel=X

NaN ElecStateLabel=X

v=0 J=2

v=0 J=7

v=0 J=7

NaN

5621.319449

5518.00699

5750.222061

4655.475479

4667.175628

5621.319449

5904.55682

5750.222061

6084.134749

5904.55682

6288.736229

4659.375574

11

15

13

11

15

13

17

1.0 ElecStateLabel=X

1.0 ElecStateLabel=X

ElecStateLabel=X

v=2 J=4

v=2 J=3 1.0 ElecStateLabel=X

v=2 J=5

v=2 J=0

NaN ElecStateLabel=X v=2 J=2

1.0 ElecStateLabel=X

1.0 ElecStateLabel=X

1.0 ElecStateLabel=X

1.0 ElecStateLabel=X v=2 J=7

1.0 ElecStateLabel=X

1.0 ElecStateLabel=X

v=2 J=6

v=2 J=8

v=2 J=1

NaN ElecStateLabel=X

v=2 J=5

v=2 J=4

cdms:a384a34a-

4739-4aa2-ae54-

4739-4aa2-ae54-

cdms:a384a34a-

4739-4aa2-ae54-

c63ee4882c8d:get cdms:8286be4e-

6d60-4659-862d-

7fd11f128228:get cdms:8286be4e-

6d60-4659-862d-

7fd11f128228:get

cdms:a384a34a-

4739-4aa2-ae54-

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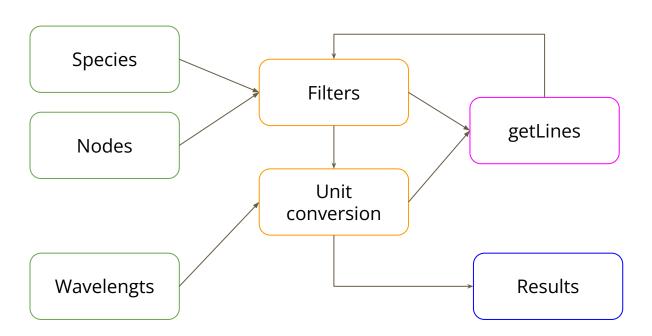
c63ee4882c8d:get

c63ee4882c8d:get cdms:a384a34a-

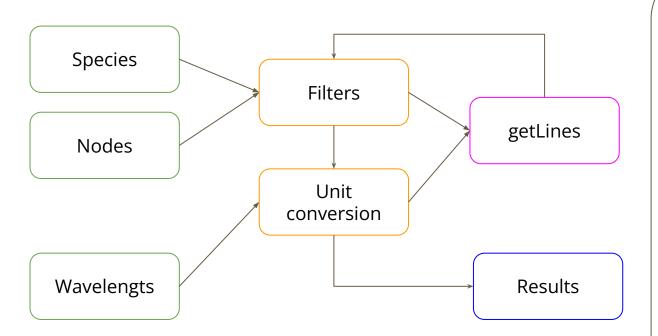
1 atomic_lines, molecular_lines = lines.getLines(lambda_min, lambda_max, species_df, nodes_df, verbose=True)

		_														
index	InchlKey	Inchi	Chemical name	Stoichiometric formula	Ordinary structural formula	Frequency	Α	Lower energy(1/cm)	Lower total statistical weight A	Lower nuclear statistical weight	Lower QNs	Upper energy(1/cm) Up	oper total statistical weight Up	per nuclear statistical weight	Upper QNs	queryToken
13	WVVLBIYUCXYYEU- JHFFFAOYSA-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- JHFFFAOYSA-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
		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- JHFFFAOYSA-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- JHFFFAOYSA-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	MVVLBIYUCXYYEU- JHFFFAOYSA-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- JHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	164050831.663	0.000659817560053	278.075338	9	1.0	ElecStateLabel=X v=0 J=4					84a34a- 954- get
64		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	•	All the	data are	fetch	ed)
		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		- no co			
8	WVVLBIYUCXYYEU- JHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	156030556.62	0.0006930428886986	416.700305	11	1.0	ElecStateLabel=X v=0 J=5			or co or cit		pt
18	WVVLBIYUCXYYEU- JHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	164521799.391	0.0006746629402928	416.700305	11	1.0	ElecStateLabel=X v=0 J=5	•	You car	n apply t	o this	, at
7	MVVLBIYUCXYYEU- JHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	154918758.314	0.0006654469491119	582.688516	13	1.0	ElecStateLabel=X			me the		
19	WVVLBIYUCXYYEU- JHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	164929208.859	0.000688338404752	582.688516	1					and colui		
6	WVVLBIYUCXYYEU- JHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	153754932.243	0.0006431487976855	775.844335	1		StateLab I=7				IIII UI	II C
20	MVVLBIYUCXYYEU- UHFFFAOYSA-N	1S/CH/h1H/q+1	Methylidynium	CH+	CH+	165272341.18	0.0006975063069331	775.844335	1		StateLabel=X I=7		conver	SIONS!!!		get
			Nitrosylium, Nitrosyl ion	NO+	NO+	139326988.819	0.3879340831149696	11.927478	1		StateLabel=X I=2	465			V-2 J-1	7fd11f128228:get

Wrapping up



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.

 \rightarrow 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.