# **Spectcol Documentation**

Release 2502\_r1

Yaye Awa BA, Marie-Lise Dubernet, Corinne Boursier

Jun 04, 2025

# Table des matières

Presentation	1
Task 1 : Discovering database species	2
Task 2 : Collision and Radiative searchTask 2.1 : Radiative searchTask 2.2 : Collisional search	<b>5</b> 5 8
Task 3 : Grouping data	10

### Presentation

Spectcol is a tool dedicated to handling XSAMS formatted data for the purpose of extracting and merging Einstein and rate coefficients from different sources.

Spectcol is an executable software, developed in Java language. The document gives a help on Spectcol's functionality and how to use it. Several versions have been developed since the beginning of the project, but the latest version is the "2502\_r1".

This application has a direct access to data from 4 databases :

- Basecol
- CDMS
- JPL Molecular Spectroscopy
- Hitran

# Task 1 : Discovering database species

When the application launches, the main window appears. If this is the first time you are launching the application or if you have installed a new version, you must first accept the terms and conditions before the main window opens.

#### Main window :

Speccorra	9.9
	Не
nport data from file	
Browse File path: path	Collision Radiative Collision & Radiative Impo
earch VAMDC databases	
tabases to search: VAMDC Nodes (You have to select a database to enable the fields below)	
Species Collision & Radiative	
earch form Selected databases	
uclear spin isomer	
olecular species InChiKey	
olecular stoichiometric formula	
n charge	
tomic symbol	
article name Submit query Cancel	
trieved Radiative data	
trieved Radiative data           Comment         Source         Structural formula Stoichiometric f         Spin	InChi key VAMDC case * Clear
rieved Radiative data Comment Source Structural formula Stoichiometric f Spin	InChi key VAMDC case + Clear Sources Energy table
rieved Radiative data Comment Source Structural formula Stoichiometric f Spin	InChi key VAMDC case * Clear Sources Energy table Rad, Trans.
rieved Radiative data Comment Source Structural formula Stoichiometric f Spin	InChi key VAMDC case * Clear Sources Energy table Rad. Trans. Partition function
rieved Radiative data Comment Source Structural formula Stoichiometric f Spin Radiative table is empty	InChi key VAMDC case * Clear Sources Energy table Rad. Trans. Partition function Export
rieved Radiative data Comment Source Structural formula Stoichiometric f Spin Radiative table is empty	InChi key VAMDC case + Clear Sources Energy table Rad. Trans. Partition function Export Group by species
rrieved Radiative data Comment Source Structural formula Stoichiometric f Spin Radiative table is empty	InChI key VAMDC case + Clear Sources Energy table Rad. Trans. Partition function Export Group by species Group by hand
trieved Radiative data Comment Source Structural formula Stoichiometric f Spin Radiative table is empty	InChI key VAMDC case * Clear Sources Energy table Rad. Trans. Partition function Export Group by speciet Group by hand QS link
trieved Radiative data  Comment Source Structural formula Stoichiometric f Spin  Radiative table is empty  trieved Collisional data	InChi key VAMDC case * Clear Sources Energy table Rad. Trans. Partition function Export Group by species Group by hand QS link
rieved Radiative data           Comment         Source         Structural formula         Stoichiometric f         Spin           Radiative table is empty         Radiative table is empty	InChi key VAMDC case * Clear Sources Energy table Rad. Trans. Partition functior Export Group by specie: Group by shand QS link
rieved Radiative data           Comment         Source         Structural formula         Stoichiometric f         Spin           Radiative table is empty         Radiative table is empty         Radiative table is empty         Radiative table is empty	InChi key VAMDC case + Clear Sources Energy table Rad. Trans. Partition function Export Group by species Group by hand QS link
rieved Radiative data           Comment         Source         Structural formula         Stoichiometric f         Spin           Radiative table is empty         Radiative table is empty	InChi key VAMDC case + Clear Sources Energy table Rad. Trans. Partition function Export Group by species Group by hand QS link . Collider s Collider I VAMDC C. + Clear Sources Energy table
rieved Radiative data           Comment         Source         Structural formula         Stoichiometric f         Spin           Radiative table is empty         Radiative table is empty	InChI key VAMDC case + Clear Sources Energy table Rad. Trans Partition functior Export Group by species Group by hand QS link Collider s Collider I VAMDC C. + Clear Sources Energy table Rate coef.
trieved Radiative data           Comment         Source         Structural formula         Stoichiometric f         Spin           Radiative table is empty	InChI key VAMDC case + Clear Sources Energy table Rad. Trans. Partition function Export Group by species Group by species Group by shand QS link Collider s Collider I VAMDC C.+ Clear Sources Energy table Rate coef. Scale rate coef.
etrieved Radiative data           Comment         Source         Structural formula         Stoichiometric f         Spin           Radiative table is empty         Radiative table is empty         Radiative table is empty         Radiative table is empty	InChI key VAMDC case + Clear Sources Energy table Rad. Trans. Partition function Export Group by species Group by species Group by shand QS link Collider s, Collider I, VAMDC C. + Clear Sources Energy table Rate coef. Scale rate coef. Export

For this first task we will use the "Search VAMDC databases" section. It enables users to select the relevant databases and to perform the queries on the selected databases. The databases must be selected before the queries forms are used. Though all VAMDC-connected databases are reachable, only CDMS, JPL, HITRAN and BASECOL are allowed for queries.

		VAMDC	Nodes	>
	Title	Description	Status	Ivold
	ACol - database	Database for coll	active	ivo://vamdc/acol
	AMBDAS: Atomic	The Atomic and	active	ivo://vamdc/amb
	AMDIS Ionization	Ionization cross	active	ivo://vamdc/amd
	Acetylene Spect	High-temperatur	active	ivo://vamdc/asd
✓	BASECOL2015:	This database, c	active	ivo://vamdc/bas
	Belgrade electro	Electron interact	active	ivo://vamdc/emo
$\checkmark$	CDMS	The Cologne Dat	active	ivo://vamdc/cdm
	Carbon Dioxide	The current vers	active	ivo://vamdc/cds
	Carbon Dioxide	The current vers	active	ivo://vamdc/cds
	Carbon Dioxide	Carbon Dioxide	active	ivo://vamdc/cds
	Carbon Dioxide	Carbon Dioxide	active	ivo://vamdc/cds
	Carbon Dioxide	The high-temper	active	ivo://vamdc/cds
	Chianti	Chianti consists	active	ivo://vamdc/chia
	GeCaSDa: Gema	Calculated line li	active	ivo://vamdc/dijo
	GhoSST	The GhoSST dat	active	ivo://vamdc/ghosst
	Hitran (VAMDC-T	HITRAN is a mol	active	ivo://vamdc/hitr
	IDEADB - Innsbr	This database co	active	ivo://vamdc/IDE
	JPL database: VA	The JPL databas	active	ivo://vamdc/jpl/v
	KIDA: Kinetic Da	KIDA is a databa	active	ivo://vamdc/kida
	MeCaSDa - Meth	Calculated line li	active	ivo://vamdc/dijo
	NIST Atomic Spe	This database nr	active	ivo://vamdc/nist/

Then we will use the "Species Search" tab, it is selected by default at startup. It allows the user to retrieve species information from the selected databases.

There are 6 query parameters. The only "exotic" one is the molecular species InChiKey. The InChI identifier describes chemical substances in terms of layers of information — the atoms and their bond connectivity, tautomeric information, isotope information, stereochemistry, and electronic charge information. It is human readable.

The InChIKey is a 25 characters long hash of an InChI identifier and as such is not human readable. It is used in VAMDC species database as an unique identifier for species.

Let's look for available isotope related to the CS molecule in the BASECOL and CDMS database. Verify that these two databases are the only checked one. You will notice that each time you select a database, the "Selected databases" box on the right side, updates accordingly, displaying the currently selected databases. Then, in the "Molecular Stoichiometric Formula" field, enter "CS".

	Species search result –											
	comment	source	structural formula	stoichiometric formula	spin	InChI key						
1	Theoretical rotational energy	BASECOL2015: VA	CS	CS		DXHPZXWIPWDXHJ-UHFFFAOYSA-N						
2	44501- v2*:CS; \$v=0-4\$	CDMS 2025-03-21	CS	CS		DXHPZXWIPWDXHJ-UHFFFAOYSA-N						
3	45501- v 2:C-13-S; \$v=0,1\$	CDMS 2025-03-21	C-13-S	CS		DXHPZXWIPWDXHJ-OUBTZVSYSA-N						
4	45502- v 2:CS-33; \$v=0,1\$	CDMS 2025-03-21	CS-33	CS		DXHPZXWIPWDXHJ-VQEHIDDOSA-N						
5	46501- v 2:CS-34; \$v=0,1\$	CDMS 2025-03-21	CS-34	CS		DXHPZXWIPWDXHJ-HQMMCQRPS						
6	46508- v 1:C-13-S-33; \$v=0\$	CDMS 2025-03-21	C-13-S-33	CS		DXHPZXWIPWDXHJ-ZDOIIHCHSA-N						
7	47501- v 2:C-13-S-34; \$v=0\$	CDMS 2025-03-21	C-13-S-34	CS		DXHPZXWIPWDXHJ-RGIGPVFXSA-N						
8	48503- v 2:CS-36; \$v=0\$	CDMS 2025-03-21	CS-36	CS		DXHPZXWIPWDXHJ-XKBLRHCCSA-N						
9	49508- v 1:C-13-S-36; \$v=0\$	CDMS 2025-03-21	C-13-S-36	CS		DXHPZXWIPWDXHJ-JOTDZXCOSA-N						

### Task 2 : Collision and Radiative search

In this task, we will search for collisional and radiative data. Click on the "Collision & Radiative search" tab. On the left side, you will notice three radio buttons that allow the user to : - Perform a radiative search, - Perform a collision search, - Perform both searches simultaneously.

If you choose Radiative, make sure that only spectroscopic databases (CDMS, JPL or HITRAN) are active. If you choose Collision, ensure that only Basecol is active. Otherwise, you will receive multiple pop-up warnings informing you that the search has failed.

### Task 2.1 : Radiative search

Once again we will look for data available for the CS molecule. Check the CDMS database and indicate "CS" as "Molecular stoichiometric formula". Submit query (and wait for a little while as it can take some time). Sometimes, there is too much data, causing the request to fail. In such cases, you need to apply additional constraints by filling in the other fields.

**Expected Result :** 

					Sp	ectcol FX							- • ×
													Help
Import data from	file												
Browse File	e path:	path							Collis	sion 🔵	Radiative Ocol	lision	& Radiative Import
Search VAMDC da	tabases												
Databases to sear	ch: VAMDC	Nodes	(You have to sele	ct a database to er	nable the	e fields below)							
Species Collisio	on & Radiative												
Brocossos	n a Radiative	Soarch fr	1700									Col	acted databases
Flocesses		Searching										CDI	AS
Collision		Nuclear s	pin isomer	_any_	-	WAVELENGTH	•			Α -			-
Radiative		Molecula	r species InChiKey			Equivalent wavele	n	Label	Label		A		
Collision & ra	diative					Upper state energ	/			1/ •			
		Molecula	r stoichiometric form	CS		Equivalent to		Label	Label	1/c	m		
						Lower state energ	/			1/ •			
						Equivalent to		Label	Label	1/c	Submit qu		
						Probability, A					Cancel		
Retrieved Radiativ	ve data	ment	Source	Structural formula	Stoichi	ometric f	Spin		InCl	hi kev		+	Clear
1	48503- v	2:CS-36	CDMS 2025-03-21	CS-36	CS		-		DXHPZXV	VIPWDXH	. DCS	<u>^</u>	Sources
2	45509- v	1*:C-13	CDMS 2025-03-21	C-13-S	CS				DXHPZXV	VIPWDXH	. DCS		Energy table
3	47501- v	2:C-13	CDMS 2025-03-21	C-13-S-34	CS				DXHPZXV	VIPWDXH	. DCS		Rad. Trans.
4	46508- v	1:C-13	CDMS 2025-03-21	C-13-S-33	CS				DXHPZXV	VIPWDXH	. DCS		Partition function
5	44511- v	1*:CS; \$	CDMS 2025-03-21	CS	CS				DXHPZXV	VIPWDXH	. DCS		Export
6	46501- v	2:CS-34	CDMS 2025-03-21	CS-34	CS				DXHPZXV	VIPWDXH	. DCS		Group by species
7	44501- v	2*·CS· \$	CDMS 2025-03-21	CS .	CS.				DXHP7XV	VIPWDXH	DCS	>~	Group by hand
Retrieved Collision	nal data	Source	Target str Targe	t st Target spin	Target	In Collider s.	Collide	er st	Collider	s Colli	ider I VAMDC C	as+	Clear
Retrieved Collision	nal data	Source	Target str Targe	t st Target spin	Target	In Collider s	. Collide	er st	Collider	s Colli	ider I VAMDC C	as+	Clear
Retrieved Collision	nal data Comment	Source	Target str Targe	t st Target spin	Target	In Collider s	. Collide	er st	Collider	s Colli	ider I VAMDC C	as⁺	Clear Sources
Retrieved Collision	nal data	Source	Target str Targe	t st Target spin	Target	In Collider s	. Collide	er st	Collider	s Colli	ider I VAMDC C	as+	Clear Sources Energy table
Retrieved Collision	nal data Comment	Source	Target str Targe	t st Target spin	Target	In Collider s	. Collide	er st	Collider	s Colli	ider I VAMDC C	as *	Clear Sources Energy table Rate coef.
Retrieved Collision	nal data	Source	Target str Targe	t st Target spin	Target	In Collider s	. Collide	er st	Collider	s Colli	ider I VAMDC C	as *	Clear Sources Energy table Rate coef. Scale rate coef.

All the available datasets appeared in the table. Thanks to the buttons on the right, it is possible to display all the informations related to the currently selected dataset :

- Sources (list of all publications related to those data )

- Energy tables ( list of levels )
- Radiative Transitions (list of transitions and values of Einstein coefficients)
- Partition function (values of partition function for different temperatures)

Take some time to try all those functionnalities. All those informations can be saved as csv files. Informations related to data sources can be exported as bibtex too.

Under the partition function button is the "Export" button. It allows the user to export the data of a dataset either as an XSAMS file or in the RADEX format. Select the data for the file labelled 48503 and export it as "Radex for LTE".

Οι	uvrir 🗸	(IT) //Bureau/to	<b>e</b> est-sur-s	Enregistre	r 🔳	- 0	×
1	!MOLECUL	-E					
2 (	CS-36	_					
3	!MOLECUL	AR WEIGHT					
4 4							
6	76	OF ENERGY LEV	ELJ				
7	!LEVEL +	- ENERGIES(CM^	-1) + WE	IGHT + El	ecStatel	_abel J v	.
8	1	0.0	1.0	X_0_0			
9	2	1.5847	3.0	X_1_0			
10	3	4.7541	5.0	X_2_0			
12	4	9.5082	7.0	X_3_0 X_4_0			
13	6	23.7698	11.0	X 5 0			
14	7	33.2771	13.0	X_6_0			
15	8	44.3684	15.0	X_7_0			
16	9	57.0437	17.0	X_8_0			
1/	10	/1.3026	19.0	X_9_0 X_10_0			
19	12	104.5701	23.0	X_10_0 X_11_0			
20	13	123.5782	25.0	X 12 0			
21	14	144.1686	27.0	X_13_0			
22	15	166.341	29.0	X_14_0			
23	16 17	190.0949	31.0	X_15_0 X_16_0			
24	18	242.3457	35.0	X 17 0			
26	19	270.8414	37.0	X_18_0			
27	20	300.9168	39.0	X_19_0			
28	21	332.5711	41.0	X_20_0			
29	22	365.8039	43.0	X_21_0 X_22_0			
31	23	437.0019	47.0	X 23 0			
32	25	474.9659	49.0	X_24_0			
33	26	514.5056	51.0	X_25_0			
34	27	555.6202	53.0	X_26_0			
35	28	598.3089	55.0	X_27_0 X_28_0			
37	30	688.4055	59.0	X 29 0			
38	31	735.8116	61.0	X_30_0			
39	32	784.7885	63.0	X_31_0			
40	33	835.3351	65.0	X_32_0			
41	34 35	881.4505 9/1 1337	6/.U 60 0	X_33_0 x 3∕ ∩			
43	36	996.3837	71.0	X 35 0			
44	37	1053.1995	73.0	X_36_0			
45	38	1111.5799	75.0	X_37_0			
46	39	1171.5238	77.0	X_38_0			
4/	4⊍ ⊿1	1233.0301	(9.0 Q1 0	X_39_0 X_40_0			
40	41	1360.7252	83.0	×_40_0 X 41 Ω			
50	43	1426.9115	85.0	X_42_0			
51	44	1494.6553	87.0	X_43_0			
	Texte bru	ıt 🗸 Largeur des	tabulation	s:8 ~	Lig 1, Col	1 ~	INS

This file can be used directly to calculate line intensities in interstellar clouds under LTE conditions.

### Task 2.2 : Collisional search

We are now back in the "Search VAMDC databases" area, where we will search for collisional data. Click on the "VAMDC Nodes" button and select "BASECOL".

Next, go to the "Collision & Radiative search" tab, select the "Collision" radio button, and proceed with the query. To find a dataset, you can specify criteria for both the target and the collider of the collision. We will search for CS data so that we can later combine the results with radiative data.

For now, let's retrieve all available data. Simply enter "CS" in the "Molecular stoichiometric formula" field.

#### **Expected result :**

					Specto	col FX						-	
													Н
nport d	lata from file												
Browse.	File path:	bath						Collision	Radiati	ve 🔵 Coll	ision	& Radiative	mp
earch V	AMDC databases												
atabase	es to search: VAMDC N	lodes	(You have to	select a database t	o enable the	fields below	1)						
Species	s search Collision & Radi	iative sear	rch										
Process	ses	Search	form							Selecte	d dat	abases	
Coll	lision			Target		Collider				BASECO	OL201	5: VAMDC-TAP	ir
Rad	liativo	Nuclea	r spin isomer	_any_	*	_any_	*						
	lision & Padiativo												
	ision & Raulative	Molecu	liar species inChik	key									
		Molecu	llar stoichiometric	formula									
		lon cha	arge										
			a maked										
		Atomic	Symbol										
		Atomic	e name					Submit que	ry Cancel	<			>
		Atomic Particle	e name					Submit que	Cancel	<			>
etrieve	d Radiative data	Atomic Particle	e name					Submit que	Cancel	<		)	>
etrieve	d Radiative data	Atomic Particle	e name Source	Structural form	Stoichiomet	ric	Spin	Submit quer	y VA	MDC case	*	Clear	>
etrieve	ed Radiative data Comme 46508- v 1:	Atomic Particle ent C-13 C	Source	Structural form C-13-S-33	<b>Stoichiomet</b> CS	ric	Spin	Submit quer	y VA DX DCS	MDC case	*	Clear Sources	>
etrieve	d Radiative data Commo 46508- v 1: 47501- v 2:	Atomic Particle ent C-13 C C-13 C	Source DMS 2025-05-2 DMS 2025-05-2	<b>Structural form</b> C-13-S-33 C-13-S-34	Stoichiomet CS CS	ric	Spin	Submit quer	y VA DX DCS DX DCS	MDC case	*	Clear Sources Energy tab	>
etrieve	d Radiative data Comm 46508- v 1: 47501- v 2: 45502- v 2:	Atomic Particle ent C-13 C C-13 C CS-3 C	Source DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2	<b>Structural form</b> C-13-S-33 C-13-S-34 CS-33	Stoichiomet CS CS CS	ric	Spin	Submit quer	y VA DX DCS DX DCS DX DCS	MDC case	•	Clear Sources Energy tab Rad. Trans	> le
etrieve	d Radiative data Commo 46508- v 1: 47501- v 2: 45502- v 2: 49508- v 1:	Atomic Particle ent C-13 C C-13 C CS-3 C C-13 C	Source DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2	Structural form C-13-5-33 C-13-5-34 C5-33 C-13-5-36 C-13-5-36 C-13-5-36	Stoichiomet CS CS CS CS	:ric	Spin	Submit quer	y VA DX DCS DX DCS DX DCS DX DCS DX DCS	MDC case		Clear Sources Energy tab Rad. Trans Partition func	> ple 5.
etriever	ed Radiative data Commo 46508- 11 47501- v 2: 45502- v 2: 49508- v 1: 48503- v 2: 48503-	Atomic Particle ent C-13 C C-13 C CS-3 C CS-3 C CS-3 C	Syntool Source DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2	Structural form C-13-5-33 C-13-5-34 C5-33 C-13-5-36 C5-36 C5-36 C5-36	Stoichiomet CS CS CS CS CS CS	ric	Spin	Submit quer	y VA DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS	MDC case		Clear Sources Energy tab Rad. Trans Partition func Export	)le s.
etriever	ed Radiative data 46508- v1: 47501- v 2: 45502- v 2: 49508- v 1: 48503- v 2: 44501- v2* 44501- v2*	Atomic Particle C-13 C C-13 C C-3 C C-13 C C-13 C C-13 C CS-3 C CS-3 C	Symbol 2 name Source DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2	Structural form C-13-5-33 C-13-5-34 CS-33 C-13-5-36 CS-36 CS CS CS CS	Stoichiomet CS CS CS CS CS CS CS CS	:ric	Spin	Submit quer	y VA DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS	MDC case		Clear Sources Energy tab Rad. Trans Partition func Export Group by spe	> ole s. :tion :cie
etriever	td Radiative data 46508- v 1: 47501- v 2: 45502- v 2: 49508- v 1: 48503- v 2: 44501- v2: 44510- v1:	Atomic Particle C-13 C C-13 C C-13 C C-13 C C-13 C C-13 C C-13 C C-13 C C:5-3 C C:5-3 C C:5-3 C C:5-3 C C:5-3 C C:5-3 C	Symbol 2 name DDMS 2025-05-2 DDMS 2025-05-2 DDMS 2025-05-2 DDMS 2025-05-2 DDMS 2025-05-2 DDMS 2025-05-2 DDMS 2025-05-2	Structural form C-13-5-33 C-13-5-34 CS-33 C-13-5-36 CS-36 CS CS CS	Stoichiomet CS CS CS CS CS CS CS CS CS	:ric	Spin	Submit quer	y VA DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS	MDC case	*	Clear Sources Energy tab Rad. Trans Partition func Export Group by spe Group by ha	> ele s. cie
etrieve	ed Radiative data	Atomic Particle C-13 C C-13 C C-3 C C-3 C C-3 C C-3 C CS: \$ C CS; \$ C	Symbol 2 name DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2	Structural form C-13-5-33 C-13-5-34 CS-33 C-13-5-36 CS-36 CS CS CS	Stoichiomet CS CS CS CS CS CS CS CS	:ric	Spin	InChI ke DXHPZXWIPW DXHPZXWIPW DXHPZXWIPW DXHPZXWIPW DXHPZXWIPW DXHPZXWIPW DXHPZXWIPW	y VA DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS	MDC case		Clear Sources Energy tab Rad. Trans Partition func Export Group by spe Group by ha	> ple s. :tio :tio
etrieve	ed Radiative data  Comme  46508-v1: 45502-v2: 49508-v1: 48503-v2: 44501-v2* 44510-v1* ed Collisional data  Comment S	Atomic Particle C-13 C C-13 C C-13 C C-13 C C-13 C C-13 C C:S; \$ C C:S; \$ C	Symbol 2 name DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 Target st	Structural form C-13-5-33 C-13-5-34 CS-33 C-13-5-36 CS-36 CS CS CS CS CS	Stoichiomet CS CS CS CS CS CS CS CS CS CS	collider s	Spin Collider s	InChi ke DXHPZXWIPW DXHPZXWIPW DXHPZXWIPW DXHPZXWIPW DXHPZXWIPW DXHPZXWIPW DXHPZXWIPW DXHPZXWIPW DXHPZXWIPW DXHPZXWIPW	y Cancel y VA DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS Collider I	MDC case	*	Clear Sources Energy tab Rad. Trans Partition func Export Group by spe Group by ha	> ple s. :tio ecie
etrieve	ed Radiative data	Atomic Particle ent C-13 C C-3 C C-3 C C-3 C C-3 C CS: S C CS; S C CS; S C	Symbol Source DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 DMS 2025-05-2 Target st Tar CS CS CS	Structural form C-13-5-33 C-13-5-34 CS-33 C-13-5-36 CS-36 CS CS CS CS CS CS	Stoichiomet CS CS CS CS CS CS CS CS CS CS CS DXHPZXW	ric Collider s	Spin Collider s	Submit quer	y VA DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS SW0 X 0G	MDC case	*	Clear Sources Energy tab Rad. Trans Partition func Export Group by spe Group by ha Clear Sources	> ole s. :tio ecie
etrieve	td Radiative data	Atomic Particle ent C-13 C C-3 C C-3 C C-3 C C-3 C C-3 C CS: S C CS: S C CS: S C COULT CCS S C C CS: S C C CS: S C C CS: S C C CS: S C C CS: S C C C CS: S C C C C C C C C C C C C C C C C C C	Symbol 2 name Source DDMS 2025-05-2 DDMS 2025-05-2 DDMS 2025-05-2 DDMS 2025-05-2 DDMS 2025-05-2 DDMS 2025-05-2 DDMS 2025-05-2 Target st Tar CS CS CS	Structural form           C-13-S-33           C-13-S-34           CS-33           C-13-S-36           CS-36           CS           GS           CS           CS           CS           CS           CS           CS           CS           CS	Stoichiomet CS CS CS CS CS CS CS CS CS CS DXHPZXW DXHPZXW	ric Collider s He He	Spin Collider s He He	Submit quer	y VA DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS SW0/X/0G SW0/X/0G	MDC case	•	Clear Sources Energy tab Rad. Trans Partition func Export Group by spe Group by ha Clear Sources Energy tab	> ple s. cie and
L 2 3 4 4 5 5 5 7 7 L 2 3	td Radiative data	Atomic Particle C-13 C C-13 C C-3 C C	Symbol a name Source DDMS 2025-05-2 DDMS 202	Structural form           C-13-5-33           C-13-5-34           C5-33           C-13-5-34           C5-36           C5-36           CS           GS           GS	Stoichiomet CS CS CS CS CS CS CS CS Target In DXHPZXW DXHPZXW DXHPZXW	rric Collider s He He Hs_25	Spin Collider s He He H2	Submit quer	y VA DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS UX DCS DX DCS UX DCS DX DCS	MDC case VAMDC C. DCS DCS DCS	*	Clear Sources Energy tab Rad. Trans Partition func Export Group by spe Group by ha Clear Sources Energy tab Bate conf	> s. tion ecie
1 2 3 4 5 6 6 7 7 1 2 3 3 4	td Radiative data	Atomic Particle C-13 C C-13 C C-3 C C-3 C C-3 C C-3 C C:S: S C C C:S: S C C:S: S C C C:S: S C C C C:S: S C C C C:S: S C C C C:S: S C C C C:S: S C C C C:S: S C C C C:S: S C	Symbol           2 name           DDMS 2025-05-2           DS 2025-05-2           DS 2025-05-2           DS 2025-05-2           DS 2025-05-2           DS 2025-05-2           DS 2025-05-2           DMS 2025-05-2           DMS 2025-05-2           DS 2025-05-2           DS 2025-05-2           DMS 2025-05-2           CS           CS           CS           CS           CS           CS           CS           CS           CS	Structural form           C-13-5-33           C-13-5-34           C5-33           C-13-5-36           CS-36           CS           GS	Stoichiomet CS CS CS CS CS CS CS CS CS CS DXHPZXW DXHPZXW DXHPZXW DXHPZXW	<b>Collider s</b> He Hs_25 Hs_25	Spin Collider s He He H2 H2	Submit quer	y Cancel y VA DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS Collider I SWQ]XJOG UFHFLCQ UFHFLCQ	MDC case VAMDC c. DCS DCS DCS DCS	*	Clear Sources Energy tab Rad. Trans Partition func Export Group by spe Group by ha Clear Sources Energy tab Rate coef	> s. tion and
Letrieve 1 2 3 4 5 6 6 7 7 1 2 3 3 4 5 5 5 5 5 5 5 5 5 5 5 5 5	td Radiative data	Atomic Particle C-13 C C-13 C C-3	Symbol           e name           DMS 2025-05-2           CS         CS           CS         CS           CS         CS	Structural form           C-13-S-33           C-13-S-34           CS-33           C-13-S-36           CS           CS	Stoichiomet CS CS CS CS CS CS CS CS CS CS CS DXHPZXW DXHPZXW DXHPZXW DXHPZXW	<b>Collider s</b> He Hs_25 Hs_25	<b>Spin</b> <b>Collider s</b> He He H2 H2 H2	Submit quer	y Cancel y VA DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS DX DCS SW0XJOG SW0JXJOG SW0JXJOG UFHFLCQ UFHFLCQ	MDC case VAMDC C. DCS DCS DCS DCS DCS DCS DCS	•	Clear Sources Energy tab Rad. Trans Partition func Export Group by spe Group by ha Group by ha Clear Sources Energy tab Rate coef Scale rate co	> ple s. cie and pef.

We can do a more precise request, by specifying the colliding species. For example we could look for data implying a CS + He collision. Enter "He" in the Atomic symbol field. There should only be **2** available collisions.

						Specto	ol FX						- 6
													H
nport da	ata from file												
rowse.	File path:	path							Collision	Radiative	Collision	n & Radiative	Impo
earch V	AMDC databases												
tabase	s to search: VAM	DC Nodes	(You have	to select a	database to	enable the f	ields below)						
Species	search Collision &	Radiative sea	irch										
rocess	es	Search	n form								Selected da	tabases	
Colli	sion			7	Farget		Collider				BASECOL20	15: VAMDC-T	AP ir
Radi	ative	Nuclea	ar spin isomer		_any_	•	_any_	•					
Colli	sion & Radiative	Moloc	ular species InCl	hiKey									
		Molect	alar species inci	likey									
		Molecu	ular stoichiomet	ric formula	CS								
		lon ch	arge										
			c cymbol				He						
		Atomi	CSVIIIDU										
		Atomi.	c symbol						Submit query	Cancel	<		>
		Particl	e name						Submit query	Cancel	< [	)	>
etrieved	d Radiative data	Particl	e name						Submit query	Cancel	< [	)	>
etrieved	d Radiative data	Atomi Particl mment	le name Source	Struct	tural form	Stoichiomet	ric f	Spin	Submit query	Cancel	MDC case *	Clea	>
etrieved	d Radiative data	Atomi Particl	le name Source	Struct	tural form	Stoichiomet	ric f	Spin	Submit query	y Cancel	MDC case *	Clea	> ar ces
etrieved	d Radiative data	Particl	le name Source	Struct	tural form	Stoichiomet	ric f	Spin	Submit query	y Cancel	MDC case +	Clea Source Energy	> ar ces table
etrieved	d Radiative data	Atomi Particl	le name Source	Struct	tural form	Stoichiomet	ric f	Spin	Submit quer	y Cancel	MDC case +	Clea Sourc Energy Rad. Tr	ar ces table rans.
etrieved	d Radiative data	Atomi Partici	le name Source	Struct	<b>tural form</b> Radiative tal	Stoichiomet	ric f	Spin	Submit query	y Cancel	MDC case +	Clea Sourd Energy Rad. Tr Partition f	> ar ces table rans. function
etrieved	d Radiative data	Atomi Particl	le name Source	Struct	<b>tural form</b> Radiative tal	<b>Stoichiomet</b> ble is empty	ric f	Spin	Submit query	y Cancel	MDC case +	Clea Source Energy Rad. Tr Partition f Expo	> ar ces table rans. function ort
etrieved	d Radiative data	Atomi Particl	le name Source	Struct	<b>tural form</b> Radiative tal	Stoichiomet	ric f	Spin	Submit query	y Cancel	MDC case +	Clea Source Energy Rad. Tr Partition f Expo Group by	> ces table rans. function ort specie
etrieved	d Radiative data	Particl	le name Source	Struct	<b>tural form</b> Radiative tal	Stoichiomet	ric f	Spin	Submit query	Y Cancel	MDC case *	Clea Source Energy Rad. Tr Partition f Expo Group by Group by	> ar ces table rans. functior ort specie: y hand
etrieveo	d Radiative data	Atomi Particl	Source	Struct	<b>tural form</b> Radiative tal	Stoichiomet	ric f	Spin	Submit query	y Cancel	MDC case +	Clea Sourd Energy Rad. Th Partition f Expo Group by Group by	> table rans. functio ort specie y hand
etrieved	d Radiative data	Atomi Particl mmment	Source	Struct	tural form Radiative tal	Stoichiomet	ric f Collider s	Spin Collider s	Submit query	( Cancel ey VA	MDC case +	Clea Sourr Energy Rad. Tr Partition f Group by Group by Group by	> ces table rans. functio ort specie y hand
strieved	d Radiative data Co d Collisional data Comment Rotational d	Atomi Particl mmment Source BASECOL2	Target st 1 CS C S C	Struct Farget st	tural form Radiative tal	Stoichiomet ble is empty Target In DXHPZXWI	ric f Collider s He	Spin Collider s	Submit query	/ Cancel y VA Collider I SW0/XJ0G	MDC case +	Clea Sourc Energy Rad. Tr Partition f Expt Group by Group by Group by Clea Sourc	> ar ces table rans. iunctio ort specie y hand
etrieved	d Radiative data Co d Collisional data Comment Rotational d Ro-vibration	Source BASECOL2 BASECOL2	Target st 1 CS CS CS	Struct Farget st 25 25	Radiative tal	Stoichiomet ble is empty Target In DXHPZXWI DXHPZXWI	ric f Collider s He He	Spin Collider s He He	Submit query	/ Cancel  y VA  Collider I SW0/X/0G SW0/X/0G	MDC case + VAMDC C. + DCS DCS	Clear Sourr Energy Rad. Tr Partition f Expt Group by Group By Grou	ar ces table rans. iunctio ort specie y hand ar ces table
etrieved etrieved	d Radiative data Co d Collisional data d Collisional data Rotational d Ro-vibration	Source BASECOL2	Source Target st 1 CS C CS C	Struct	tural form Radiative tal	Stoichiomet ble is empty Target In DXHPZXWI	ric f Collider s He He	Spin Collider s He He	Submit query	Cancel y VA Collider I SW0/XJ0G	MDC case * VAMDC C. * DCS DCS	Clear Sourr Energy Rad. Th Partition f Experg Group by Group by Group by Group by Group by Group by Group by Group by Group by Group by Rate c	> ar ces table rans. runction ort specie y hand ar ces table coef.
etrieved 1 2	d Radiative data Co d Collisional data Rotational d Ro-vibration	Atomi Particl	Target st 1 CS C	Struct	Radiative tal	Stoichiomet ble is empty DXHPZXWI DXHPZXWI	ric f Collider s He He	Spin Collider s He He	Submit query	Y Cancel  y VA  Collider I SW0JXJ0G	MDC case * VAMDC c. * DCS DCS	Clea Sourr Energy Rad. Tr Partition f Expery Group by Group by Group by Clea Sourr Energy Rate c Scale rat	> ar ces table rans. runction ort specie y hand ar ces table coef. e coef.

Once again, for each dataset, it is possible to display and export the data it contains as a CSV file :

- Sources
- Energy table of both target and collider
- Rate coefficients
- Whole file as XSAMS file

# Task 3 : Grouping data

A very convenient feature of this application is the possibility to merge data from Basecol and from a spectroscopic database. The software will identify equivalent levels in energy tables according to their quantum numbers. Then it will produce a table containing levels existing in both tables, using energy values from the spectroscopic database. Finally, it will give rate and Einstein coefficients for the levels available after merging the tables.

The first thing to do is looking for CS data available in spectroscopic databases. We did that in task 2.1. Secondly, we have to look for CS by He collisions, as we did in task 2.2.

#### **Expected result :**

						Spectcol FX										-
port data from f	ïle															
rowse File	e path: path									• C	ollision	Rad	liative	Colli	ision (	& Radiative
earch VAMDC dat	tabases															
tabases to searc	th: VAMDC Nodes ()	ou have to select	t a databas	e to enable the fi	elds be	low)										
pecies search	Collision & Radiative search															
ocesses	Search form											Sele	cted data	bases		
Collision												CDM	s			
Dediative	Nuclear spin	isomer	_any_	•	WAVE	LENGTH 👻	to		A -							
Radiative	Molecular st	oecies InChiKev			Equival	ent wavelength	Label	Label		A						
Collision & Ra	diative				Upper s	state energy	to		1/cm -							
	Molecular st	oichiometric formu	la CS		Equival	ent to	Label	Label	1/c	m						
					Lower s	state energy	to		1/cm -							
					Equival	ent to	Label	Label	1/c	" Submi	auerv					
											e query					
trieved Radiativ	e data				Probab	ility, A	to			Cance						
trieved Radiativ	e data Comment	Source	St	ructural formula	Stoid	ility, A	. s	oin		Cance	l key		VAMDC	case	•	Clear
trieved Radiativ	e data Comment 47501- v 2:C-13-5-34.	Source	St 1 14: C-13	<b>ructural formula</b> 3-5-34	Probab Stoid CS	ility, A	. S	oin	DXH	Cancel InCh PZXWIPW	l key DXHJ-RGIGI	P DC	VAMDC CS	case	•	Clear Sources
rrieved Radiativ	e data Comment 47501- v 2:C-13-S-34. 44510- v1*:CS; \$v=	<b>Source</b> CDMS 2025-05-2 CDMS 2025-05-2	<b>St</b> 1 14: C-13 1 14: CS	<b>ructural formula</b> 3-S-34	Stoid CS CS	ility, A	. S	oin	DXH	Cancel InCh PZXWIPW PZXWIPW	<b>I key</b> DXHJ-RGIGI DXHJ-UHFF	P DC	VAMDC SS	case	•	Clear Sources Energy tab
rieved Radiativ	e data Comment 47501- v 2:C-13-5-34. 44510- v1*:C5; \$v= 44511- v1*:C5; \$v=2	Source CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2	<b>St</b> 1 14: C-13 1 14: CS 1 14: CS	ructural formula -S-34	Stoid CS CS CS	ility, A	. S	bin	DXH DXH DXH	Cancel InCh PZXWIPW PZXWIPW PZXWIPW	I key DXHJ-RGIGI DXHJ-UHFF DXHJ-UHFF	P DC F DC F DC	VAMDC CS CS CS	case	•	Clear Sources Energy tab Rad. Tran
rieved Radiativ	e data           Comment           47501- v 2:C-13-5-34.           44510- v1*:CS; Sv=           44511- v1*:CS; Sv=2           44501- v2*:CS; Sv=0	Source CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2	St           1 14:         C-1:           1 14:         CS           1 14:         CS           1 14:         CS	ructural formula 3-S-34	Probab Stoid CS CS CS CS	ility, A	. S	bin	DXH DXH DXH DXH	Cancel InCh PZXWIPW PZXWIPW PZXWIPW PZXWIPW	I key DXHJ-RGIGI DXHJ-UHFF DXHJ-UHFF DXHJ-UHFF	P DC F DC F DC F DC	VAMDC S S S S S	case		Clear Sources Energy tab Rad. Tran Partition fund
trieved Radiativ	e data Comment 47501 v 2:C-13-S-34. 44510 v 1*:CS; Sv= 44511 v 1*:CS; Sv=2 44501 v 2*:CS; sv=0 45502 v 2:CS-33; Sv	Source CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2	<b>st</b> 1 14: C-13 1 14: CS 1 14: CS 1 14: CS 1 14: CS-3	ructural formula 3-5-34 33	Probab Stoid CS CS CS CS CS CS	ility, A	. <b>S</b> I	bin		Cancel InCh PZXWIPW PZXWIPW PZXWIPW PZXWIPW	I key DXHJ-RGIGI DXHJ-UHFF DXHJ-UHFF DXHJ-UHFF DXHJ-VQEH	P DC F DC F DC F DC I DC	VAMDC 25 25 25 25 25 25	case		Clear Sources Energy tat Rad. Tran Partition fund Export
etrieved Radiativ	e data           Comment           47501 · v 2:C-13-S-34.           44510 · v1*:CS; \$v=           44511 · v1*:CS; \$v=           44501 · v2*:CS; \$v=           44502 · v2:CS-33; \$v=           45508 · v1:C1-3S-33.           45508 · v1:C1-3S-33.	Source           CDMS 2025-05-2	St           114:         C-13           114:         CS           114:         CS           114:         CS           114:         CS           114:         CS           114:         CS	ructural formula -5-34 33 -5-33	Probab Stoid CS CS CS CS CS CS CS CS	chiometric for	. <b>S</b>	bin		Cancel InCh PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW	I key DXHJ-RGIGI DXHJ-UHFF DXHJ-UHFF DXHJ-UHFF DXHJ-VQEH DXHJ-ZDOII	P DC F DC F DC F DC I DC	VAMDC 25 25 25 25 25 25 25 25 25	case		Clear Sources Energy tat Rad. Tran Partition fun Export Group by spo
trieved Radiativ	e data 47501- v 2:C-13-S-34, 44510- v1*:CS; \$v= 44510- v1*:CS; \$v=2 44502- v2:CS; 3v=0 45502- v 2:CS-33; \$v 46508- v 1:C-13-S-33, 46501- v 2:CS-34; \$v	Source           CDMS 2025-05-2	St           1 14:         C-12           1 14:         CS           1 14:         CS           1 14:         CS           1 14:         CS-12           1 14:         CS-12           1 14:         CS-12           1 14:         CS-12	ructural formula 1-5-34 33 1-5-33 34	Probab Stoid CS CS CS CS CS CS CS CS CS CS	chiometric for	. S	bin	DXH DXH DXH DXH DXH DXH DXH DXH	Cancel InCh PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW	I key DXHJ-RGIGI DXHJ-UHFF DXHJ-UHFF DXHJ-VQEH DXHJ-ZDOII DXHJ-ZDOII DXHJ-RQMI	P DC F DC F DC F DC I DC I DC I DC	VAMDC 25 25 25 25 25 25 25 25	case		Clear Sources Energy tal Rad. Tran Partition fun Export Group by spe Group by h
trieved Radiativ	e data           Comment           47501 · v 2:C-13-5-34.           44510 · v1*:CS; \$v=           44511 · v1*:CS; \$v=           44502 · v2:CS; \$v=           44502 · v2:CS; \$v=           44504 · v1*:CS; \$v=           45504 · v1:C-13-5-33.           46501 · v2:CS-34; \$v           46501 · v2:CS-34; \$v	Source CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2	St           1 14:         C-13           1 14:         C5           1 14:         C5           1 14:         C5-3           1 14:         C5-3           1 14:         C5-3	ructural formula 1-5-34 33 3-5-33 34	Probab Stoid CS CS CS CS CS CS CS CS	hiometric for	. <b>S</b>	bin	DXH DXH DXH DXH DXH	Cancel InCh PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW	I key DXHJ-RGIGI DXHJ-UHFF DXHJ-UHFF DXHJ-VQEH DXHJ-VQEH DXHJ-ZDOII DXHJ-HQM1	P DC F DC F DC I DC I DC I DC	VAMDC 25 25 25 25 25 25 25 25 25	case		Clear Sources Energy tat Rad. Tran Partition fun Export Group by spi Group by he
trieved Radiativ	e data           Comment           47501 · v 2:C-13-5-34.           44510 · v1*:CS; \$v=2.           44501 · v1*:CS; \$v=0.           44502 · v2:CS; \$v=0.           45502 · v2:CS; \$v=0.           45508 · v1:C-13-5-33.           46501 · v2:CS:S4; \$v           46501 · v2:CS:S4; \$v           46502 · v2:CS:S4; \$v	Source CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2	St           1 14:         C-13           1 14:         CS           1 14:         CS           1 14:         CS           1 14:         CS-3           1 14:         CS-3           7arget stru.         Struget stru.	ructural formula -5-34 33 -5-33 34 Target stoic	Probab Stoid CS CS CS CS CS CS CS CS CS CS CS CS CS	hiometric for	Collider str	oin Col	DXH DXH DXH DXH DXH DXH	Cancel InCh PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW	I key DXHJ-RGIGI DXHJ-UHFF DXHJ-UHFF DXHJ-VQEH DXHJ-VQEH DXHJ-ZDOII DXHJ-ZDOII DXHJ-HQM!	P DC F DC F DC F DC I DC I DC I DC	VAMDC 25 25 25 25 25 25 25 25 25 25 25 25 25	case DC Case		Clear Sources Energy tat Rad. Tran Partition fun- Export Group by spi Group by h-
trieved Radiativ trieved Collision Rotation	e data	Source CDMS 2025-05-2 Source 1 BASECOL201 C	St           1 14:         C-13           1 14:         CS           1 14:         CS           1 14:         CS-13           1 14:         CS-13	ructural formula J-S-34 J-S-33 J-S-33 J-S-33 J-S-33 J-S-33 J-S-33 J-S-33 J-S-34	Probab Stoid CS CS CS CS CS CS CS Tar	hiometric for Target InCh DXHPZXWIP	Collider str He	oin Col He	DXH DXH DXH DXH DXH DXH	Cancel InCh PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW Colli	I key DXHJ-RGIGI DXHJ-UHFF DXHJ-UHFF DXHJ-VQEH DXHJ-VQEH DXHJ-ZDOII DXHJ-HQMI . Collider SWQJXJOU	2 DC F DC F DC I DC I DC I DC I DC	VAMDC 25 25 25 25 25 25 25 25 25 25 25 25 25	case DC Case	• (	Clear Sources Energy tat Rad. Tran Partition fun Export Group by spr Group by hr Clear Sources
trieved Radiativ trieved Collision Rotation Ro-vibra	e data  Comment  47501 v 2:(-13-5-34, 44510 v 1*:(C5; sv=., 44510 v 1*:(C5; sv=.), 44501 v 2*:(C5; sv=.), 45502 v 2:(C5-33; sv, 46508 v 1:(-13-5-33, 46508 v 1:(-13-5-34, 4508 v 1:(-13-5) v 1:(-13	Source CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 Source Sou	St           1 14:         C-1i           1 14:         CS           5         S	ructural formula 1-5-34 33 3-5-33 34 4 Target stoic CS CS	Probab Stoid CS CS CS CS CS CS CS Tar	Target InCh DXHPZXWIP DXHPZXWIP	Collider str He He	oin Col He He	DXH DXH DXH DXH DXH DXH DXH	Cancel InCh PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW Colli	I key DXHJ-RGIGI DXHJ-UHFF DXHJ-UHFF DXHJ-VQEH DXHJ-ZDOII DXHJ-ZDOII DXHJ-ZDOII DXHJ-HQMI • Collider SWQJXJ00 SWQJXJ00	P DC F DC F DC I DC I DC I DC	VAMDC :5 :5 :5 :5 :5 :5 :5 :5 :5 :5 :5 :5 :5	case DC Case		Clear Sources Energy tal Rad. Tran Partition fum Export Group by sp Group by h Clear Sources Energy tal
trieved Radiativ trieved Collision Rotation Ro-vibra	e data  Comment  47501- v 2:C-13-5-34  44510- v1*:C5; \$v=  44510- v1*:C5; \$v=  44500- v1*:C5; \$v=  45502- v 2:C5-33; \$v  46501- v 2:C5-34; \$v  al data  Comment  al de=xcitation of CS by H	Source CDMS 2025-05-2 BASECOL201 CBASECOL201 C	St           1 14:         C-11           1 14:         CS           1 14:         CS           1 14:         CS-3           1 14:         CS-3           1 14:         CS-3           S         S	ructural formula 1-5-34 33 1-5-33 34 Target stoic CS CS	Probab Stoid CS CS CS CS CS CS CS CS Tar	Target InCh DXHPZXWIP DXHPZXWIP	Collider str He He	nin Col He He	DXH DXH DXH DXH DXH DXH DXH DXH	InCh PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW Colli	I key DXHJ-RGIGI DXHJ-UHFF DXHJ-UHFF DXHJ-VQEH DXHJ-ZDOII DXHJ-ZDOII DXHJ-ZDOII DXHJ-ZDOII DXHJ-HQMF . Collider SWQJXJOI SWQJXJOI	2 DC F DC F DC I DC I DC I DC I DC	VAMDC 25 25 25 25 25 25 25 25 25 25 25 25 25	case DC Case		Clear Sources Energy tai Rad. Tran Partition fum Export Group by sp Group by h Clear Sources Energy tai Rate cole
trieved Radiativ trieved Collision Rotation Ro-vibra	e data           Comment           47501 v 2:C-13-5-34.           44510- v1*:CS; \$v=           44511- v1*:CS; \$v=           44501- v2*:CS; \$v=           44501- v2*:CS; \$v=           45508- v1:C-13-5-33.           46501- v2:CS-34; \$v           44501- v2:CS-34; \$v           44501- v2:CS-34; \$v           addata           Comment           al de-excitation of CS by He           tional excitation of CS by H	Source Source Source Source BASECOL201 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 CDMS 2025-05-2 Source BASECOL201 C	St           114:         C-13           114:         CS           114:         CS           114:         CS-3           114:         CS-3           114:         CS-3           114:         CS-3	ructural formula 1-5-34 3-5-33 3-4 Target stoic CS CS	Stoid CS CS CS CS CS CS CS CS Tar	Target InCh DXHPZXWIP DXHPZXWIP	Collider str He He	Din Col He He	DXH DXH DXH DXH DXH DXH DXH	InCh PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW PZXWIPW Colli	I key DXHJ-RGIGI DXHJ-UHFF DXHJ-UHFF DXHJ-UHFF DXHJ-ZDOII DXHJ-ZDOII DXHJ-ZDOII DXHJ-ZDOII DXHJ-ZDOII DXHJ-ZDOII DXHJ-ZDOII SWQJZJOI SWQJZJOI	2 DC F DC F DC F DC F DC M DC InC	VAMDC 25 25 25 25 25 25 25 25 25 25 25 25 25	Case DC Case		Clear Sources Energy tat Rad, Tran Partition fun Export Group by spi Group by spi Group by spi Clear Sources Energy tat Rate coel Scale rate c

The "Group by hand" and "Group by species" buttons can be used for merging. The former will let the user choose manually which datasets he wants to merge. The latter will search in the collision datasets the ones whose collider corresponds to the currently selected transitions dataset.

The link between species will be performed thanks to the InChIKey value.

Click on the radiative dataset labelled "47501", then click on "Group by species". A window will appear with no corresponding collisional set. Indeed none of them uses the same InChIKey, which means it is a different **CS** isotope.

Now select the dataset labelled 44501. There are now 2 corresponding datasets.

						Pr	oces	ses group						- 0	×
Select a	a row from Tra	nsition	table	and either	Collision tab	ole or Sc	alec	Collision ta	ble						
Radiativ	es														
	Comme	nt		Source	Structural	formula	Sto	ichiometric fo	or 9	Spin	InChI key		VAI	MDC case	+
2	44510- v1*:CS	; \$v=	CDMS	2025-05-23 1	. CS		CS				DXHPZXWIPWDX	HJ	DCS		
7	44501- v2*:CS	; \$v=0	CDMS	2025-05-23 1	. CS		CS				DXHPZXWIPWDX	HJ	DCS		
8	44511- v1*:CS	; \$v=2	CDMS	2025-05-23 1	. CS		CS				DXHPZXWIPWDX	HJ	DCS		
Collision	IS														
	Comment	Sou	irce	Target str	Target sto	Target s	pin	Target InC	Collider st	Collider st.	Collider spin	Colli	der In	VAMDC c	as +
1	Rotational de	BASECO	DL20	CS	CS			DXHPZXWIP	He	He		SWQJ	XJOGL	DCS	
2	Ro-vibrationa	BASECO	DL20	CS	CS			DXHPZXWIP	He	He		SWQJ	XJOGL	DCS	
Scaled C	Collisions														
	Comment	Sou	irce	Target str	Target sto	Target s	spin	Target InC	Collider st	Collider st.	Collider spin	Colli	der In	VAMDC c	as *
						No	cont	ent in table							
													SI	now selecti	on

You will notice that all the radiative datasets with a similar InChIKey have been selected as well.

Now we can merge data. You have to select one radiative and one collisional dataset and click on "Show selection". We will use the dataset labelled **44501** in CDMS, with v=0-4. These rotational data corresponds to those found in the Basecol datasets labelled **"Rotational de-excitation of CS by He"**. The merging can be made on one among the three Basecol datasets.

A new window will show the energy tables for the radiative set and the collisional set where you can choose the quantum numbers.

			Energy	able group				- •	×
Select	the relevant o	quantum numb	pers and	VAMDC cases					
QNs: VAMDO	kronigParity cases: ODC	F pari	ty 🔽 v	asSym Ele	ecSta	ateLa	bel	✓ J _ F1	
Spectr	o DB - energy ta	ble							
Index	Energy []	Degeneracy	asSym	ElecStatel abel	F	E1	1	kronigParity	na
1	0.0	1.0	ussym	X			0	ki olingi ulity	-
2	1.6342	3.0		X			1		
3	4.9025	5.0		X			2		
4	9.8048	7.0		х			3		
5	16.3411	9.0		x			4		
6	24.5113	11.0		х			5		
7	34.3152	13.0		x			6		
8	45.7525	15.0		х			7		
9	58.8231	17.0		х			8		
10	73.5267	19.0		х			9		
11	89.8631	21.0		х			10		
12	107.8318	23.0		х			11		~
<									2
Baseco	l - energy table								
Index	Energy [1	Degeneracy	asSym	ElecStateLabel	F	F1	J	kronigParity	pa
1	0.0			Х			0		Â
2	1.634164			х			1		
3	4.90246			Х			2		
4	9.804818			Х			3		
5	16.34114			Х			4		
6	24.51129			Х			5		
7	34.3151			Х			6		
8	45.75237			Х			7		
9	58.822862			х			8		
10	73.52631			Х			9		
11	89 86241			X			10		>
								Ok Cano	el

You will be able to choose manually which quantum numbers will be used to identify similar levels in each table.

You can click on one or several columns to choose the quantum numbers. Here we will choose the rotational quantum number J and v.

The result is a new energy table containing levels available in both original tables. All related informations are provided too (Einstein and rate coefficients, sources values). You have multiple export functionnalities

so that you can use those merged data easily.

						М	atchi	ng result								-		×
St	ate er	nergy	and	quantum i	numbers													
	In	dex		Ene	rgy [1/cm]	D	egene	eracy	asS	/m	Ele	cSt	ateLabel	F	F1	J	kre	onig
1				0.0		1.0										0		^
2				1.6342	1	3.0										1		
3				4.9025	i	5.0										2		
4				9.8048		7.0										3		~
		- (U - )																>
Ка	te co	efficie	ents															
11	F1	12	F2	10.0	20.0	40	0.0	60.0		80	0.0		100.0		120	.0	1	40.
	1	1	1	2.519E-1	.1 2.251E-11	2.107	E-11	2.059E-11	L 2.	042	E-11	2	.039E-11	2.0	)45E	-11	2.05	3
3	1	1	1	1.489E-1	.1 1.41E-11	1.405	E-11	1.5E-11	1.	627	E-11	1	.759E-11	1.8	886E-	-11	2.00	3
	2	1	1	3.655E-1	.1 3.351E-11	3.184	E-11	3.139E-11	L 3.	136	E-11	3	.155E-11	3.1	185E-	-11	3.22	1
1	1	1	1	3.281E-1	.2 3.338E-12	3.52E	-12	3.66E-12	3.	789	E-12	3	.924E-12	4.0	)68E	-12	4.21	7~
																		2
Eir	nstein	coef	ficicie	ents														
Up	per le	evel	Low	er level	Frequency	[MHz]	Eins	stein coef	f [1/s	1	Lo	g (i	ntensity)		l	Jnce	rtain	ity
2			1		48990.9549		1.74	916398201	1888.	3	3.62	32		(	0.002	2		Â
}			2		97980.9533		1.67	922779209	9845.	2	2.72	52		(	0.002	23		
Ļ			3		146969.0287		6.07	112231993	3073.	2	2.20	55		(	0.002	26		
			4		195954.2109		1.49	230450983	3603.	:	1.84	26		(	0.001	16		~
																		>
Co	llider	state	e ener	gy and qu	iantum numbe	rs												
	In	dex		Ene	rgy [1/cm]	D	egene	eracy	F	J	j	к	Карра	L	м	par	ity	S
L				0.0					C	.0				0				0.0
											_			_				>
хро	rt																	
k				Energy	Rat	e coeffi	ci	Finstein	coeff	icie		Co	llider ene	av	Save	as C	sv	
				Linergy		e coem		Emotern	coch				and chericite	97	5470			