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# **Spectcol Documentation**

*Release 2502\_r1*

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# 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".

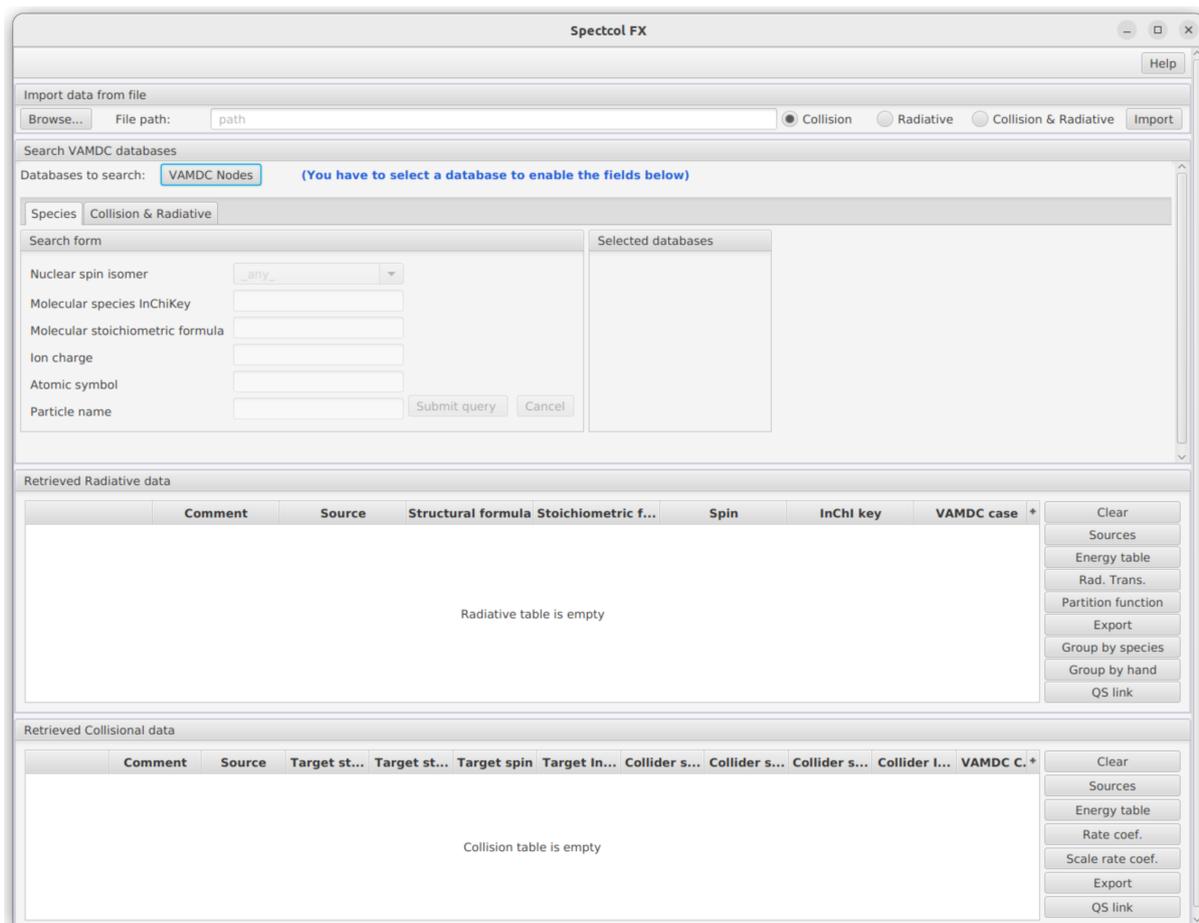
This application has a direct access to data from 4 databases :

- Basecol
- CDMS
- JPL Molecular Spectroscopy
- Hitran

## Task 1 : Discovering database species

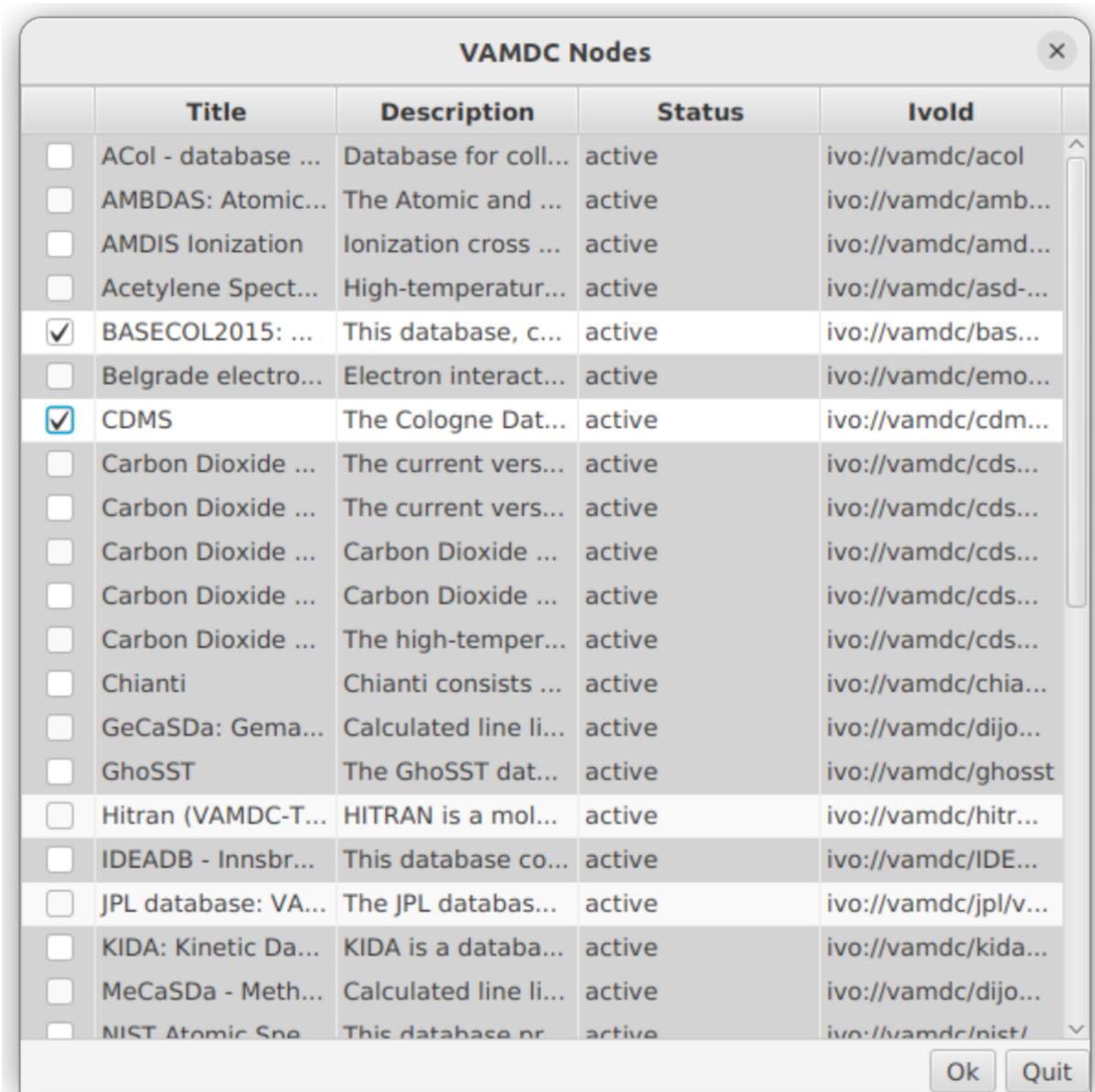
When the application launches, the main window appears. If this is the first time you are launching the application or if you have installed a new version, you must first accept the terms and conditions before the main window opens.

### Main window :



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.

### Expected result :



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”.

**Expected result :**

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- v 2*: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-ZDOIHCCHA-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 :

The screenshot shows the Spectcol FX interface with the following details:

- Search VAMDC databases:** Databases to search: VAMDC Nodes (You have to select a database to enable the fields below)
- Species:** Collision & Radiative
- Processes:** Radiative (selected)
- Search form:**
  - Nuclear spin isomer:
  - Molecular species InChiKey:
  - Molecular stoichiometric form...:
  - WAVELENGTH:    A
  - Equivalent waven...:   A
  - Upper state energy:   1/...
  - Equivalent to:   1/cm
  - Lower state energy:   1/...
  - Equivalent to:   1/cm
  - Probability, A:
- Retrieved Radiative data:**

	Comment	Source	Structural formula	Stoichiometric f...	Spin	InChI key	VAMDC case
1	48503- v 2:CS-36...	CDMS 2025-03-21 ...	CS-36	CS		DXHPZXWIPWDXH...	DCS
2	45509- v1*:C-13...	CDMS 2025-03-21 ...	C-13-5	CS		DXHPZXWIPWDXH...	DCS
3	47501- v 2:C-13...	CDMS 2025-03-21 ...	C-13-5-34	CS		DXHPZXWIPWDXH...	DCS
4	46508- v 1:C-13...	CDMS 2025-03-21 ...	C-13-5-33	CS		DXHPZXWIPWDXH...	DCS
5	44511- v1*:CS; \$...	CDMS 2025-03-21 ...	CS	CS		DXHPZXWIPWDXH...	DCS
6	46501- v 2:CS-34...	CDMS 2025-03-21 ...	CS-34	CS		DXHPZXWIPWDXH...	DCS
7	44501- v2*:CS; \$...	CDMS 2025-03-21 ...	CS	CS		DXHPZXWIPWDXH...	DCS
- Retrieved Collisional data:**

Comment	Source	Target str...	Target st...	Target spin	Target In...	Collider s...	Collider st...	Collider s...	Collider I...	VAMDC Cas*
Collision table is empty										

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 fonctionnalités. 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”.

**Expected result :**

```

Ouvrir  [+]  lte  Enregistrer  [≡]  [–]  [□]  [×]
~/Bureau/test-sur-s...

1 !MOLECULE
2 CS-36
3 !MOLECULAR WEIGHT
4 48.0
5 !NUMBER OF ENERGY LEVELS
6 76
7 !LEVEL + ENERGIES(CM^-1) + WEIGHT + ElecStateLabel_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
11  4         9.5082        7.0     X_3_0
12  5        15.8468        9.0     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
17 10        71.3026       19.0     X_9_0
18 11        87.1448       21.0     X_10_0
19 12       104.5701       23.0     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       190.0949       31.0     X_15_0
24 17       215.43         33.0     X_16_0
25 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
30 23       400.6143       45.0     X_22_0
31 24       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
36 29       642.5709       57.0     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       887.4505       67.0     X_33_0
42 35       941.1337       69.0     X_34_0
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
47 40      1233.0301       79.0     X_39_0
48 41      1296.0977       81.0     X_40_0
49 42      1360.7252       83.0     X_41_0
50 43      1426.9115       85.0     X_42_0
51 44      1494.6553       87.0     X_43_0

Texte brut  Largeur des tabulations : 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 :

The screenshot shows the Spectcol FX interface with the following data:

**Retrieved Radiative data**

	Comment	Source	Structural form...	Stoichiometric ...	Spin	InChI key	VAMDC case
1	46508- v 1:C-13-...	CDMS 2025-05-2...	C-13-S-33	CS		DXHPZXWIPWDX...	DCS
2	47501- v 2:C-13-...	CDMS 2025-05-2...	C-13-S-34	CS		DXHPZXWIPWDX...	DCS
3	45502- v 2:CS-3-...	CDMS 2025-05-2...	CS-33	CS		DXHPZXWIPWDX...	DCS
4	49508- v 1:C-13-...	CDMS 2025-05-2...	C-13-S-36	CS		DXHPZXWIPWDX...	DCS
5	48503- v 2:CS-3-...	CDMS 2025-05-2...	CS-36	CS		DXHPZXWIPWDX...	DCS
6	44501- v2*:CS; \$...	CDMS 2025-05-2...	CS	CS		DXHPZXWIPWDX...	DCS
7	44510- v1*:CS; \$...	CDMS 2025-05-2...	CS	CS		DXHPZXWIPWDX...	DCS

**Retrieved Collisional data**

	Comment	Source	Target st...	Target st...	Target spin	Target In...	Collider s...	Collider s...	Collider s...	Collider I...	VAMDC C...
1	Rotational d...	BASECOL2...	CS	CS		DXHPZXW...	He	He		SWQJXJOG...	DCS
2	Ro-vibration...	BASECOL2...	CS	CS		DXHPZXW...	He	He		SWQJXJOG...	DCS
3	Rotational e...	BASECOL2...	CS	CS		DXHPZXW...	Hs_2s	H2	PARA	UFHFLCQ...	DCS
4	Rotational e...	BASECOL2...	CS	CS		DXHPZXW...	Hs_2s	H2	ORTHO	UFHFLCQ...	DCS
5	Ro-vibration...	BASECOL2...	CS	CS		DXHPZXW...	Hs_2s	H2	PARA	UFHFLCQ...	DCS
6	Ro-vibration...	BASECOL2...	CS	CS		DXHPZXW...	Hs_2s	H2	ORTHO	UFHFLCQ...	DCS

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.

### Expected result :

The screenshot shows the Spectcol FX application window. At the top, there are options to import data from a file (Browse..., File path: path) and search VAMDC databases. The search form includes fields for Nuclear spin isomer, Molecular species InChIKey, Molecular stoichiometric formula (set to CS), Ion charge, Atomic symbol (set to He), and Particle name. The search form is set to 'Collision & Radiative' search. Below the search form, there are two data tables: 'Retrieved Radiative data' and 'Retrieved Collisional data'. The radiative data table is empty, while the collisional data table contains two rows of data. The collisional data table has columns for Comment, Source, Target st..., Target st..., Target spin, Target In..., Collider s..., Collider s..., Collider s..., Collider I..., and VAMDC C. The first row has a comment 'Rotational d...', source 'BASECOL2...', target st... 'CS', target st... 'CS', target spin 'DXHPZXWI...', target In... 'He', collider s... 'He', collider s... 'He', collider s... 'SWQJXJOG...', and VAMDC C. 'DCS'. The second row has a comment 'Ro-vibration...', source 'BASECOL2...', target st... 'CS', target st... 'CS', target spin 'DXHPZXWI...', target In... 'He', collider s... 'He', collider s... 'SWQJXJOG...', and VAMDC C. 'DCS'.

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

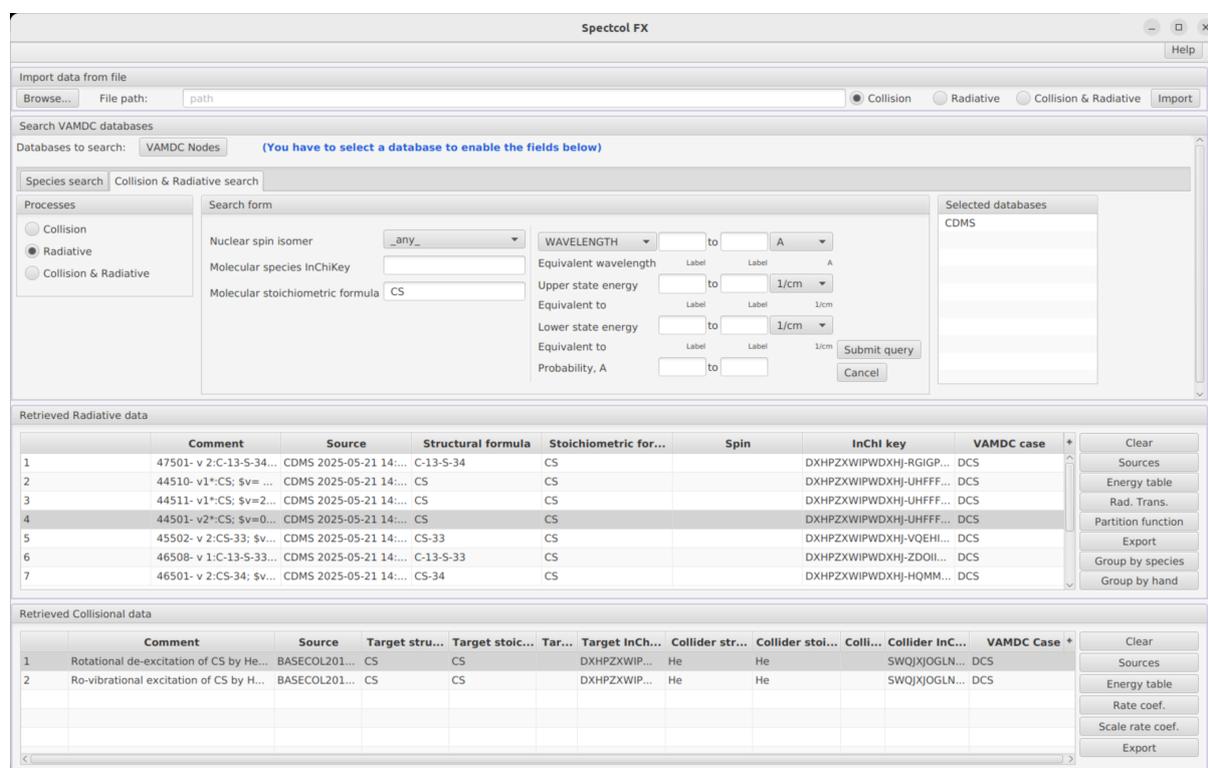
- Sources
- Energy table of both target and collider
- Rate coefficients
- Whole file as XSAMS file

## 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 :



The screenshot shows the Spectcol FX software interface. The top section is for importing data from a file. Below that is a search form for VAMDC databases. The search criteria include: Processes (Collision, Radiative, Collision & Radiative), Nuclear spin isomer (set to \_any\_), Molecular species InChIKey, and Molecular stoichiometric formula (set to CS). The search results are displayed in two tables: Retrieved Radiative data and Retrieved Collisional data.

	Comment	Source	Structural formula	Stoichiometric for...	Spin	InChI key	VAMDC case
1	47501- v 2:C-13-S-34...	CDMS 2025-05-21 14:...	C-13-S-34	CS		DXHPZXWIPWDXHJ-RGIGP...	DCS
2	44510- v1*:CS; \$v=...	CDMS 2025-05-21 14:...	CS	CS		DXHPZXWIPWDXHJ-UHFFF...	DCS
3	44511- v1*:CS; \$v=2...	CDMS 2025-05-21 14:...	CS	CS		DXHPZXWIPWDXHJ-UHFFF...	DCS
4	44501- v2*:CS; \$v=0...	CDMS 2025-05-21 14:...	CS	CS		DXHPZXWIPWDXHJ-UHFFF...	DCS
5	45502- v 2:CS-33; \$v...	CDMS 2025-05-21 14:...	CS-33	CS		DXHPZXWIPWDXHJ-VQEH...	DCS
6	46508- v 1:C-13-S-33...	CDMS 2025-05-21 14:...	C-13-S-33	CS		DXHPZXWIPWDXHJ-ZDOL...	DCS
7	46501- v 2:CS-34; \$v...	CDMS 2025-05-21 14:...	CS-34	CS		DXHPZXWIPWDXHJ-HQMM...	DCS

	Comment	Source	Target stru...	Target stoic...	Tar...	Target InCh...	Collider str...	Collider sto...	Colli...	Collider InC...	VAMDC Case
1	Rotational de-excitation of CS by He...	BASECOL201...	CS	CS		DXHPZXWIP...	He	He		SWQJXOGLN...	DCS
2	Ro-vibrational excitation of CS by H...	BASECOL201...	CS	CS		DXHPZXWIP...	He	He		SWQJXOGLN...	DCS

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 collisional 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.

### Expected result :

Processes group

Select a row from Transition table and either Collision table or Scaled Collision table

Radiatives

	Comment	Source	Structural formula	Stoichiometric for...	Spin	InChI key	VAMDC case	+
2	44510- v1*:CS; \$v= ...	CDMS 2025-05-23 1...	CS	CS		DXHPZXWIPWDXHJ-...	DCS	
7	44501- v2*:CS; \$v=0...	CDMS 2025-05-23 1...	CS	CS		DXHPZXWIPWDXHJ-...	DCS	
8	44511- v1*:CS; \$v=2...	CDMS 2025-05-23 1...	CS	CS		DXHPZXWIPWDXHJ-...	DCS	

Collisions

	Comment	Source	Target str...	Target sto...	Target spin	Target InC...	Collider st...	Collider st...	Collider spin	Collider In...	VAMDC cas *
1	Rotational de...	BASECOL20...	CS	CS		DXHPZXWIP...	He	He		SWQJXJOG...	DCS
2	Ro-vibrationa...	BASECOL20...	CS	CS		DXHPZXWIP...	He	He		SWQJXJOG...	DCS

Scaled Collisions

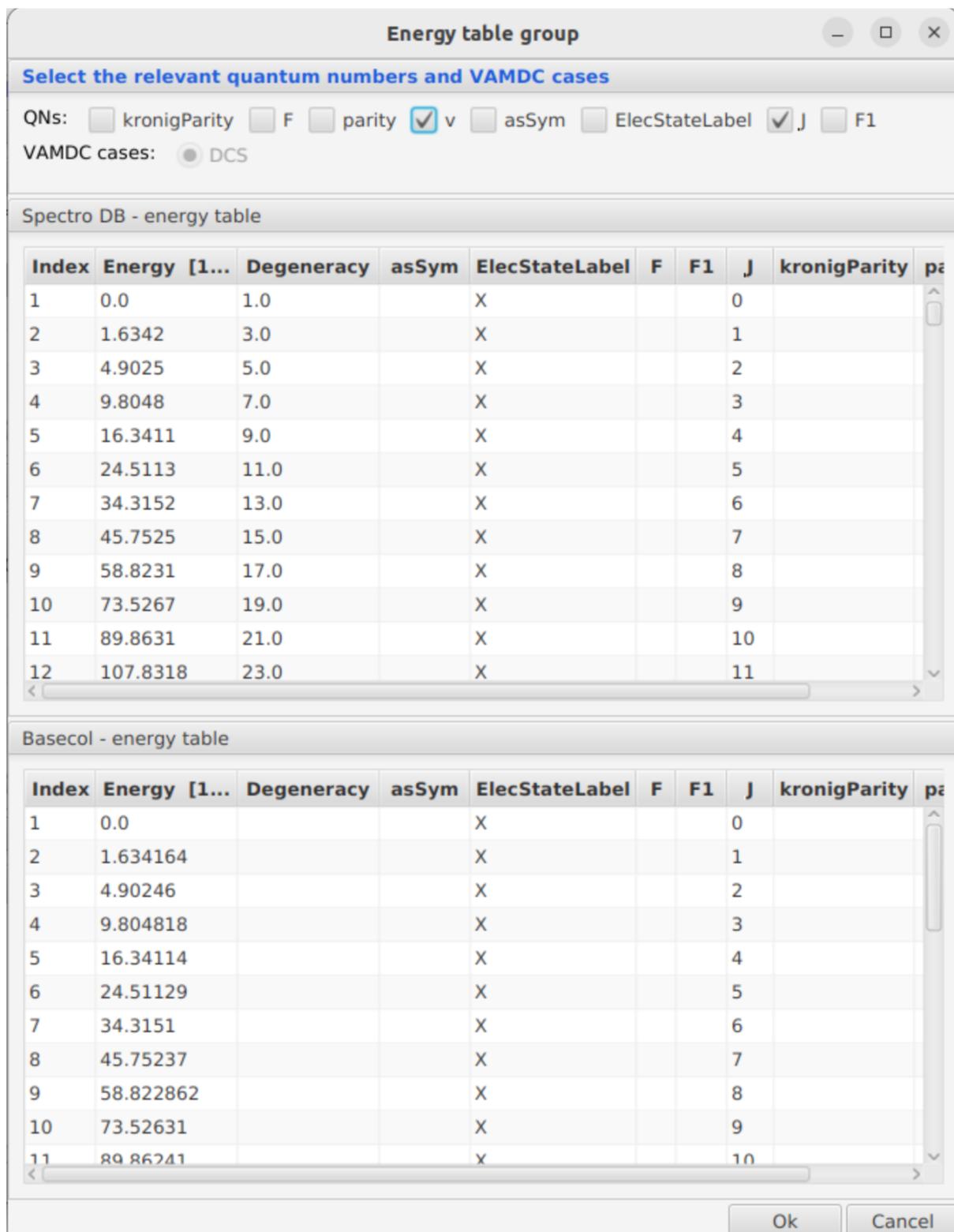
	Comment	Source	Target str...	Target sto...	Target spin	Target InC...	Collider st...	Collider st...	Collider spin	Collider In...	VAMDC cas *
No content in table											

Show selection

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.



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 functionalities

so that you can use those merged data easily.

### Expected result :

Matching result
- □ ×

▼ State energy and quantum numbers

Index	Energy [1/cm]	Degeneracy	asSym	ElecStateLabel	F	F1	J	kronic
1	0.0	1.0					0	
2	1.6342	3.0					1	
3	4.9025	5.0					2	
4	9.8048	7.0					3	

▼ Rate coefficients

I1	F1	I2	F2	10.0	20.0	40.0	60.0	80.0	100.0	120.0	140.0
2	1	1	1	2.519E-11	2.251E-11	2.107E-11	2.059E-11	2.042E-11	2.039E-11	2.045E-11	2.053E-11
3	1	1	1	1.489E-11	1.41E-11	1.405E-11	1.5E-11	1.627E-11	1.759E-11	1.886E-11	2.003E-11
3	2	1	1	3.655E-11	3.351E-11	3.184E-11	3.139E-11	3.136E-11	3.155E-11	3.185E-11	3.221E-11
4	1	1	1	3.281E-12	3.338E-12	3.52E-12	3.66E-12	3.789E-12	3.924E-12	4.068E-12	4.217E-12

▼ Einstein coefficients

Upper level	Lower level	Frequency [MHz]	Einstein coeff [1/s]	Log (intensity)	Uncertainty
2	1	48990.9549	1.74916398201888...	-3.6232	0.002
3	2	97980.9533	1.67922779209845...	-2.7252	0.0023
4	3	146969.0287	6.07112231993073...	-2.2055	0.0026
5	4	195954.2109	1.49230450983603...	-1.8426	0.0016

▼ Collider state energy and quantum numbers

Index	Energy [1/cm]	Degeneracy	F	J	j	K	Kappa	L	M	parity	S
1	0.0			0.0				0			0.0

Export

\*  Energy  Rate coeffici...  Einstein coefficie...  Collider energy

\*  Save as Radex  Save as Xsams