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".

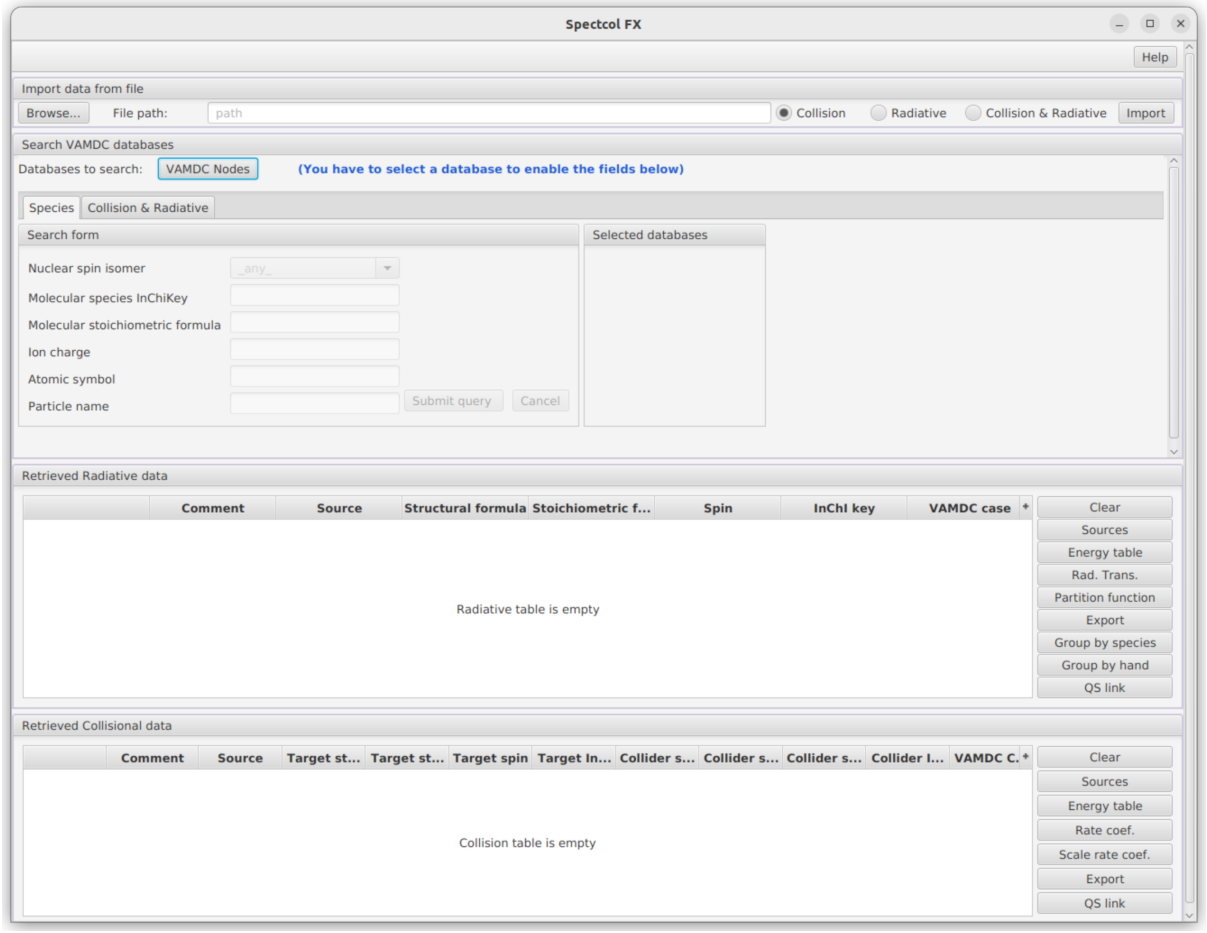
This application has a direct access to data from 4 databases :

- Basecol
- CDMS
- JPL Molecular Spectroscopy
- Hitran

Task 1 : Discovering database species

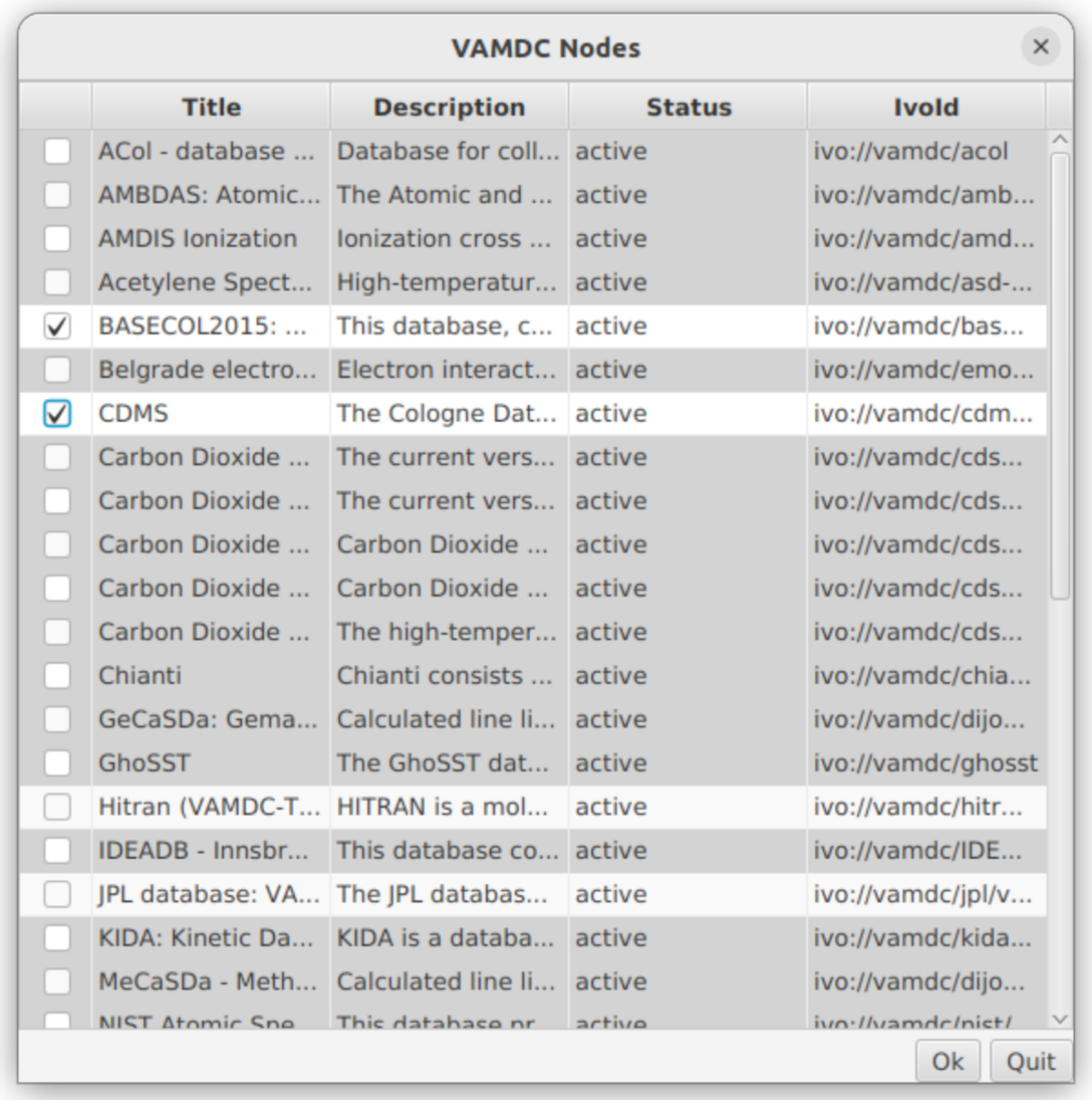
When the application launches, the main window appears. If this is the first time you are launching the application or if you have installed a new version, you must first accept the terms and conditions before the main window opens.

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 :



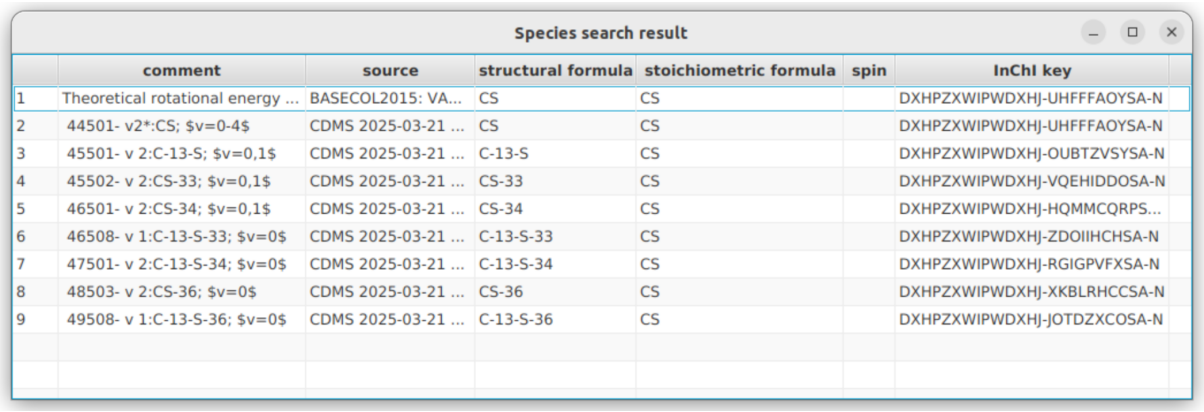
Then we will use the “Species Search” tab, it is selected by default at startup. It allows the user to retrieve species information from the selected databases.

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- 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

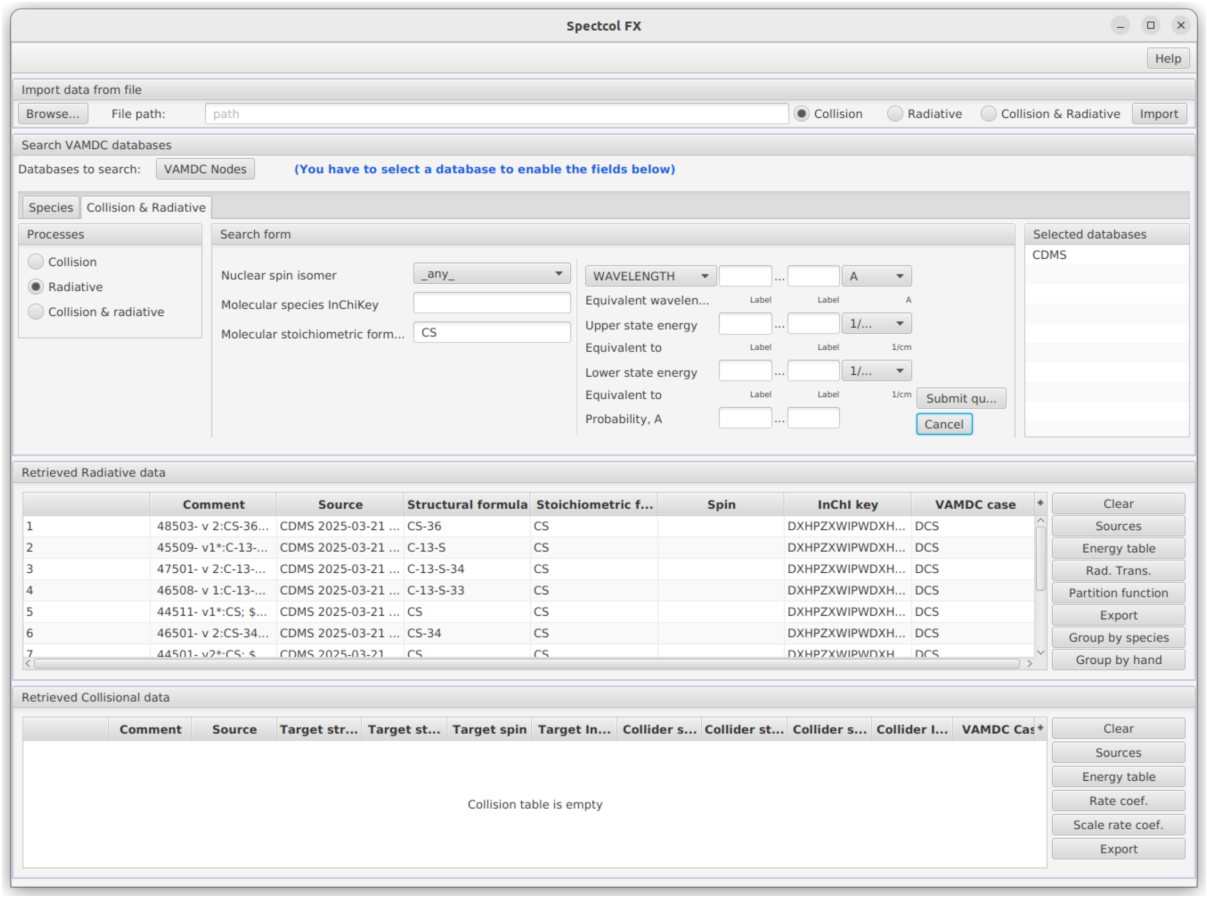
In this task, we will search for collisional and radiative data. Click on the “Collision & Radiative search” tab. On the left side, you will notice three radio buttons that allow the user to : - Perform a radiative search, - Perform a collision search, - Perform both searches simultaneously.

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 :



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 :

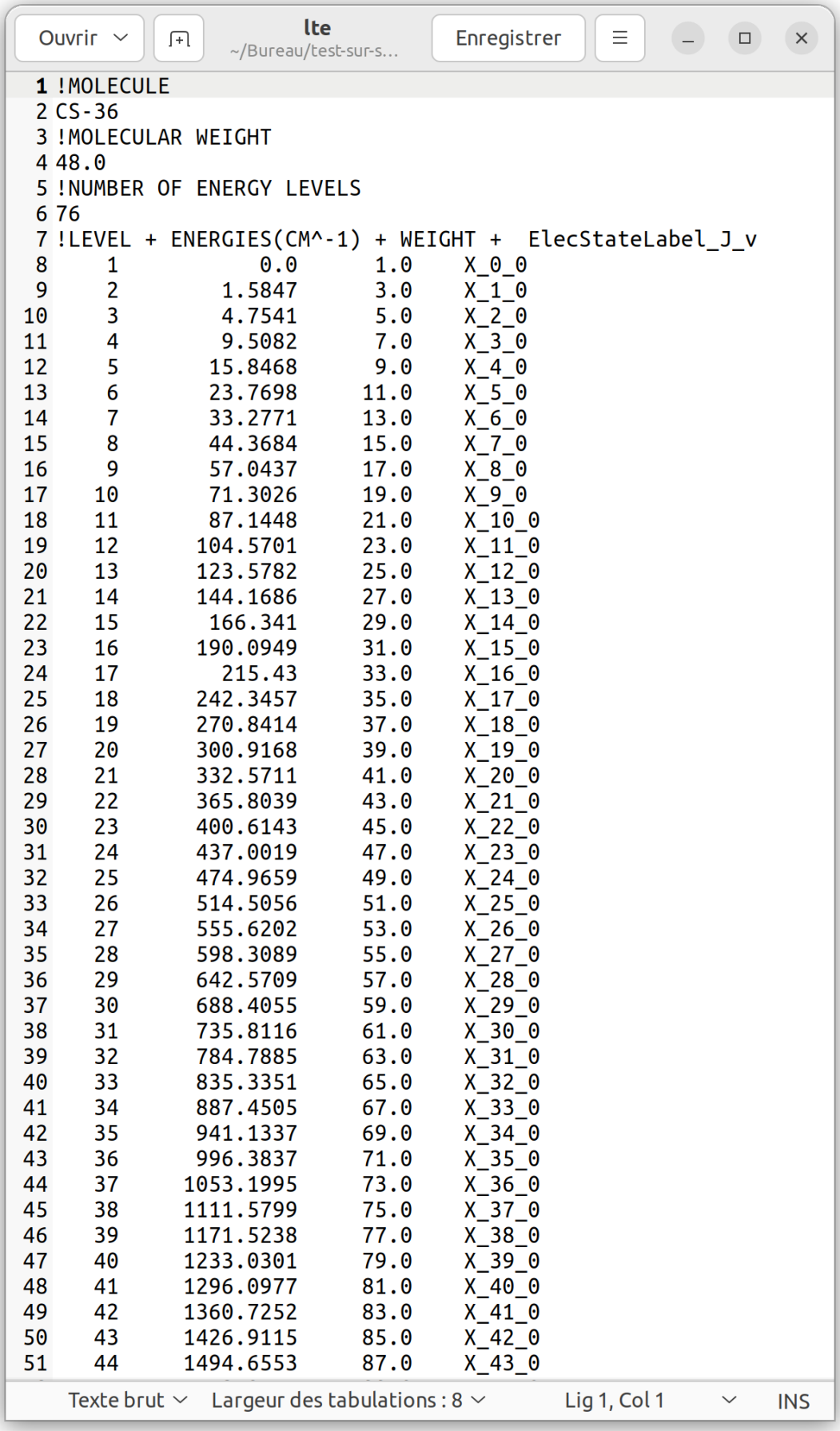
— Sources (list of all publications related to those data)

— 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”.

Expected result :




```
!MOLECULE
CS-36
!MOLECULAR WEIGHT
48.0
!NUMBER OF ENERGY LEVELS
76
!LEVEL + ENERGIES(CM^-1) + WEIGHT +  ElecStateLabel_J_v
     1            0.0       1.0    X_0_0
     2         1.5847       3.0    X_1_0
     3         4.7541       5.0    X_2_0
     4         9.5082       7.0    X_3_0
     5        15.8468       9.0    X_4_0
     6        23.7698      11.0    X_5_0
     7        33.2771      13.0    X_6_0
     8        44.3684      15.0    X_7_0
     9        57.0437      17.0    X_8_0
    10        71.3026      19.0    X_9_0
    11        87.1448      21.0    X_10_0
    12       104.5701      23.0    X_11_0
    13       123.5782      25.0    X_12_0
    14       144.1686      27.0    X_13_0
    15        166.341      29.0    X_14_0
    16       190.0949      31.0    X_15_0
    17         215.43      33.0    X_16_0
    18       242.3457      35.0    X_17_0
    19       270.8414      37.0    X_18_0
    20       300.9168      39.0    X_19_0
    21       332.5711      41.0    X_20_0
    22       365.8039      43.0    X_21_0
    23       400.6143      45.0    X_22_0
    24       437.0019      47.0    X_23_0
    25       474.9659      49.0    X_24_0
    26       514.5056      51.0    X_25_0
    27       555.6202      53.0    X_26_0
    28       598.3089      55.0    X_27_0
    29       642.5709      57.0    X_28_0
    30       688.4055      59.0    X_29_0
    31       735.8116      61.0    X_30_0
    32       784.7885      63.0    X_31_0
    33       835.3351      65.0    X_32_0
    34       887.4505      67.0    X_33_0
    35       941.1337      69.0    X_34_0
    36       996.3837      71.0    X_35_0
    37      1053.1995      73.0    X_36_0
    38      1111.5799      75.0    X_37_0
    39      1171.5238      77.0    X_38_0
    40      1233.0301      79.0    X_39_0
    41      1296.0977      81.0    X_40_0
    42      1360.7252      83.0    X_41_0
    43      1426.9115      85.0    X_42_0
    44      1494.6553      87.0    X_43_0
```

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

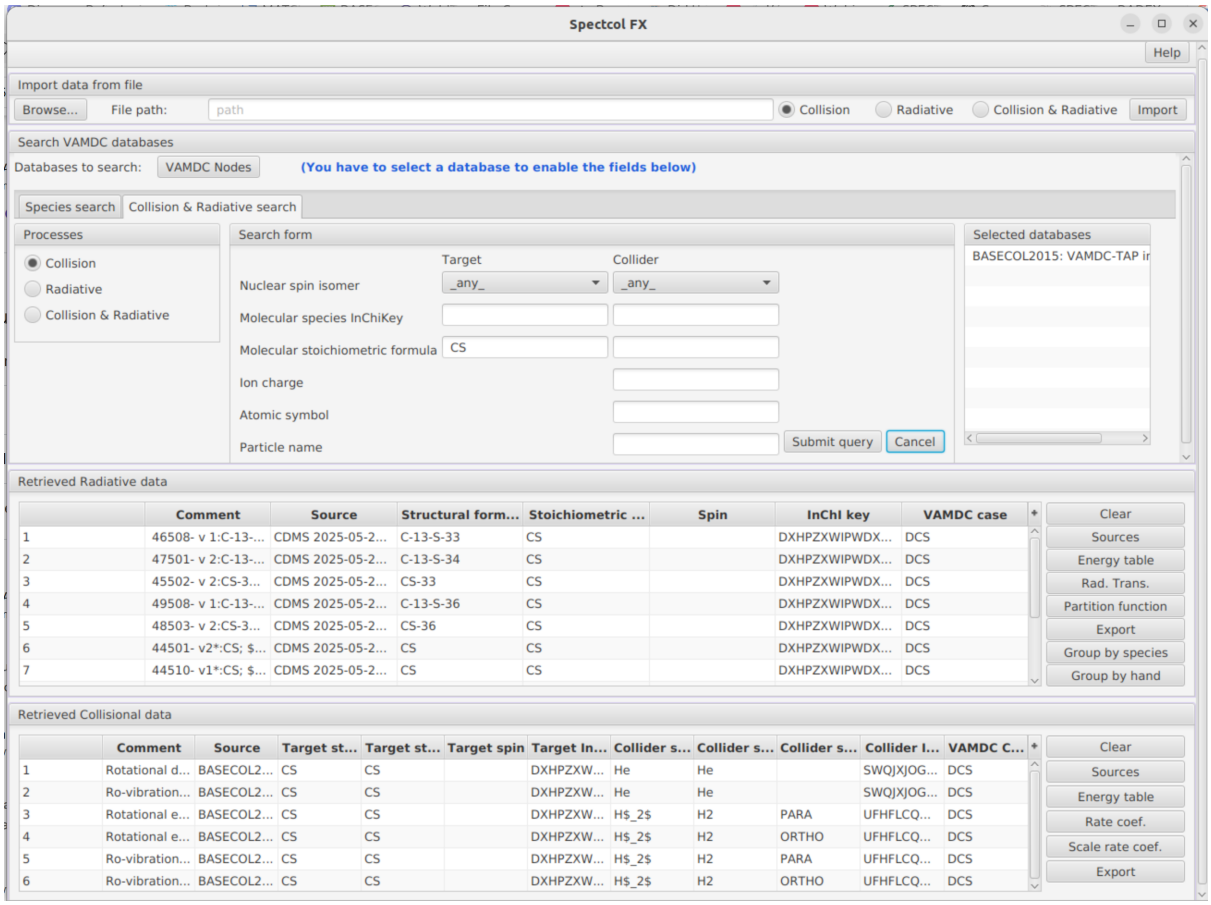
Task 2.2 : Collisional search

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.

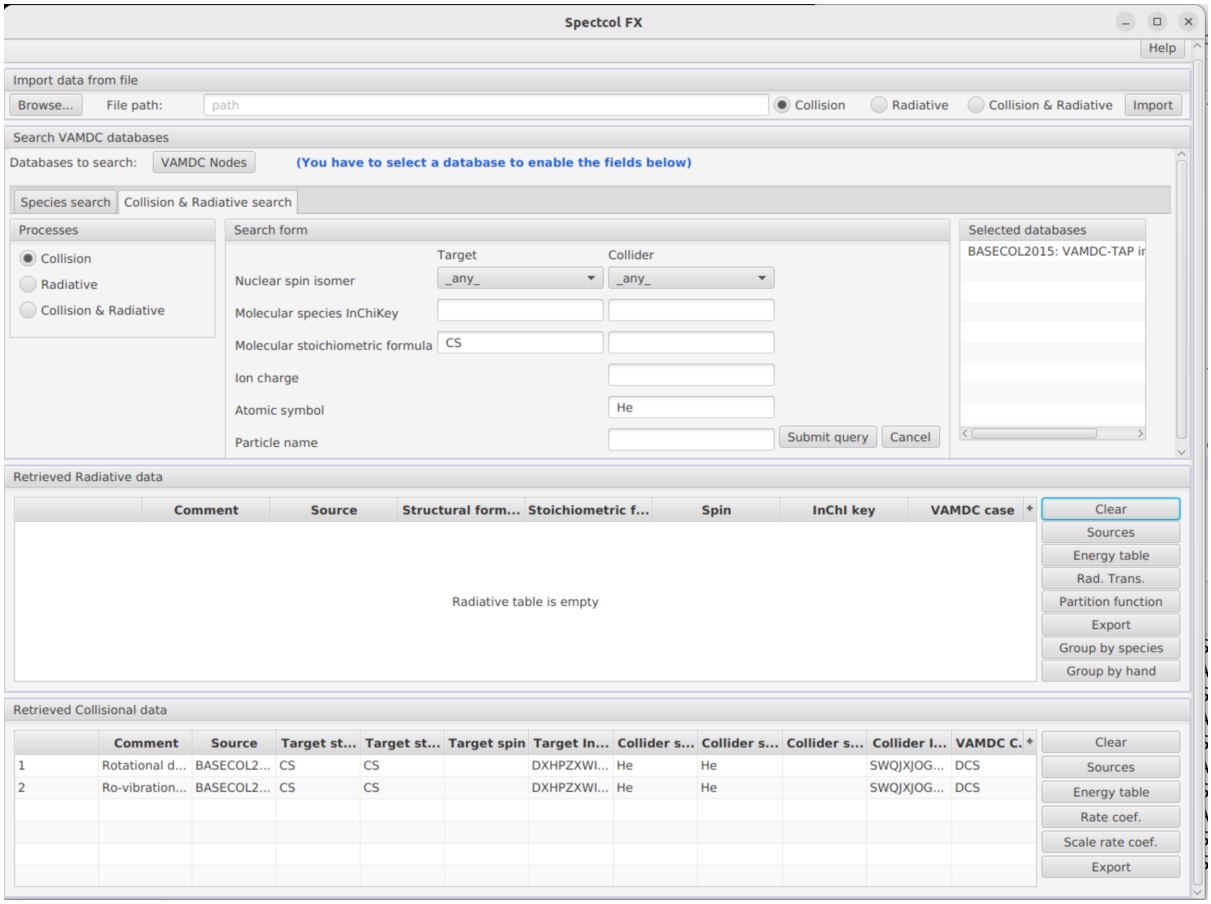
For now, let's retrieve all available data. Simply enter "CS" in the "Molecular stoichiometric formula" field.

Expected result :



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 :



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

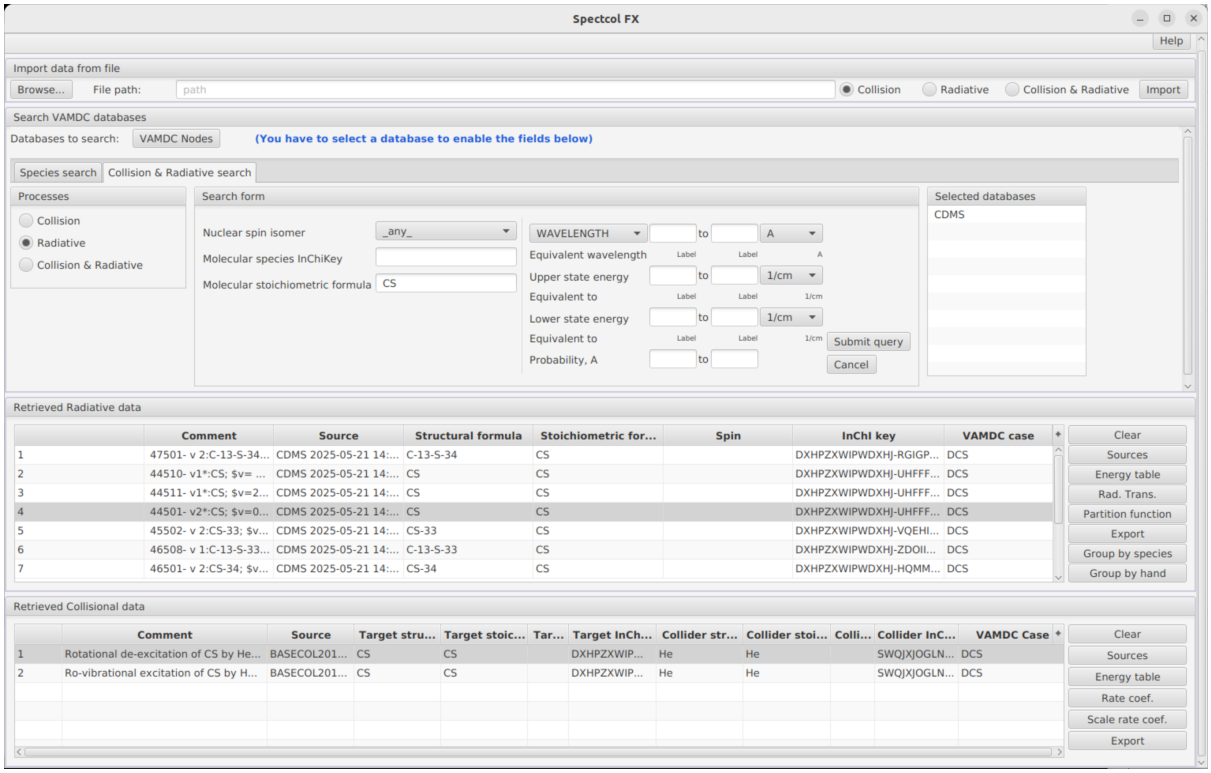
- Sources
- Energy table of both target and collider
- Rate coefficients
- Whole file as XSAMS file

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 :



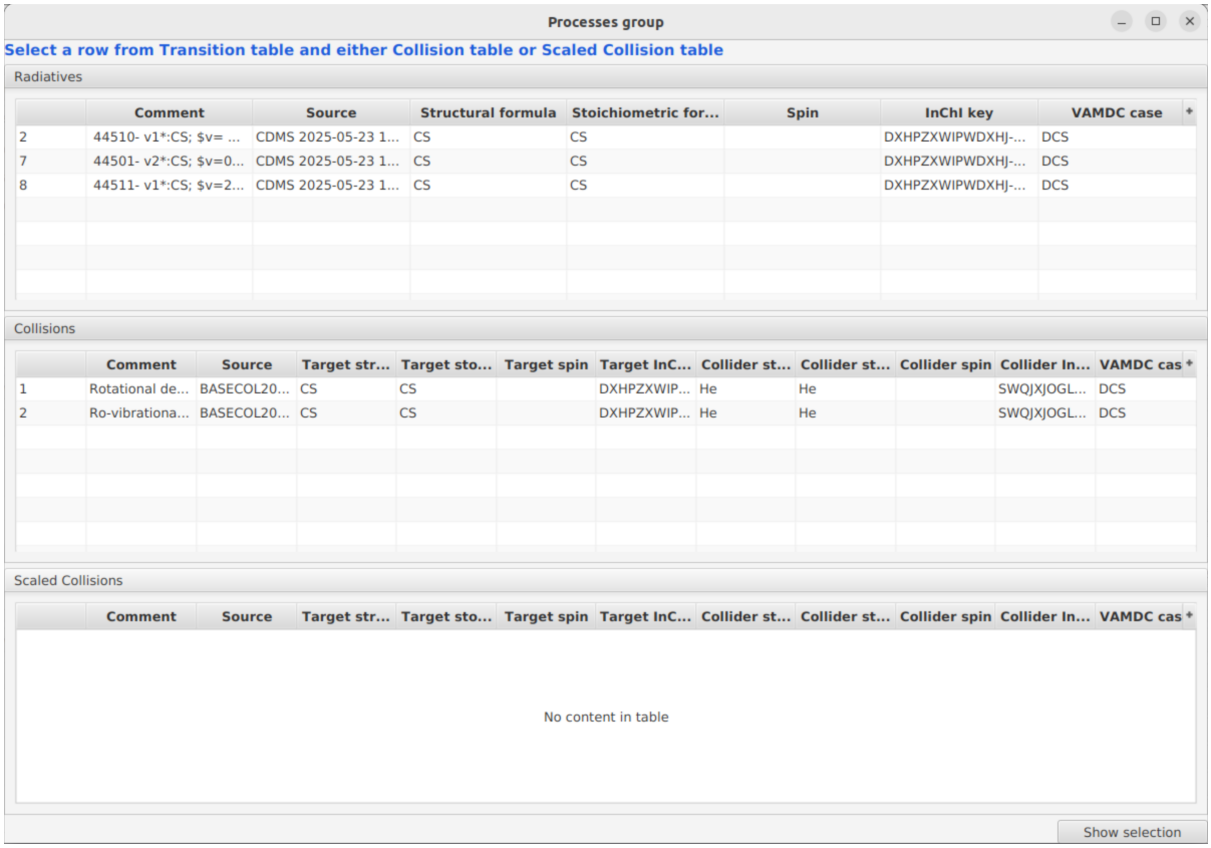
The “Group by hand” and “Group by species” buttons can be used for merging. The former will let the user choose manually which datasets he wants to merge. The latter will search in the collision datasets the ones whose collider corresponds to the currently selected transitions dataset.

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.

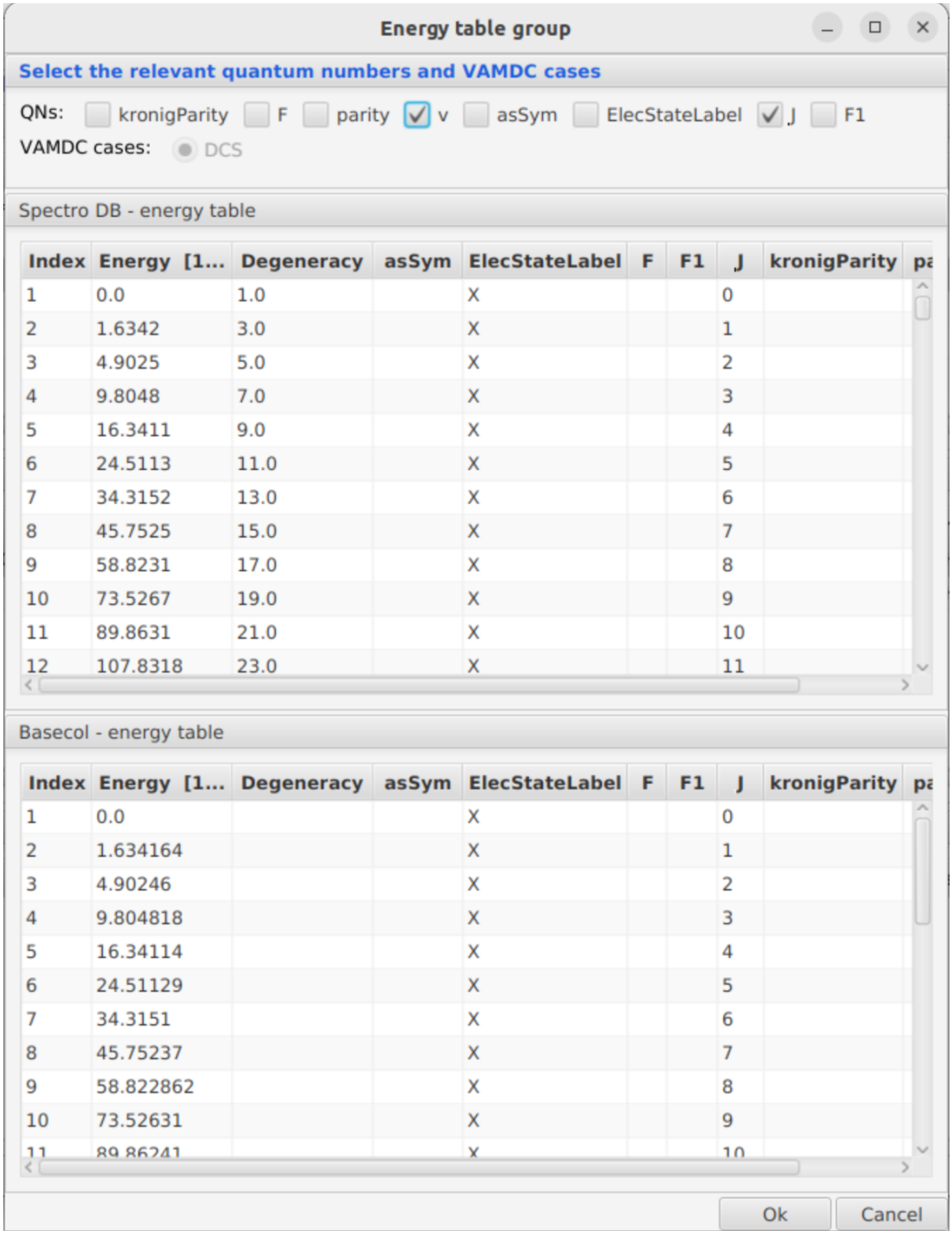
Expected result :



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 functionnalities

so that you can use those merged data easily.

Expected result :