



e-infrastructure

User's guide to SPECTCOL

Document Information

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Type of document: software documentation

Status: release

Distribution: public

Work package: WP8

Version: 11.09

Document code:

Directory and file name: http://www.vamdc.org/documents/software/SPECTCOL_guide_v11.09.pdf

Abstract: This document is a guide to the tool for the manipulation of VAMDC-XSAMS formatted data for the purpose of extracting and merging Einstein and rate coefficients from different sources.

Version History

Version	Date	Modified By	Description of Change
V0.1	01/06/11	Ljerka Nenadović	first draft

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Acknowledgements

VAMDC is funded under the "Combination of Collaborative Projects and Coordination and Support Actions" Funding Scheme of The Seventh Framework Program. Call topic: INFRA-2008-1.2.2 Scientific Data Infrastructure. Grant Agreement number: 239108.

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Introduction

This document is a guide to the SPECTCOL tool for the manipulation of VAMDC-XSAMS formatted data for the purpose of extracting and merging Einstein and rate coefficients from different sources. For more information on the XML schema used visit the VAMDC Standards Documentation page at <http://www.vamdc.org/documents/standards/>

Configuration

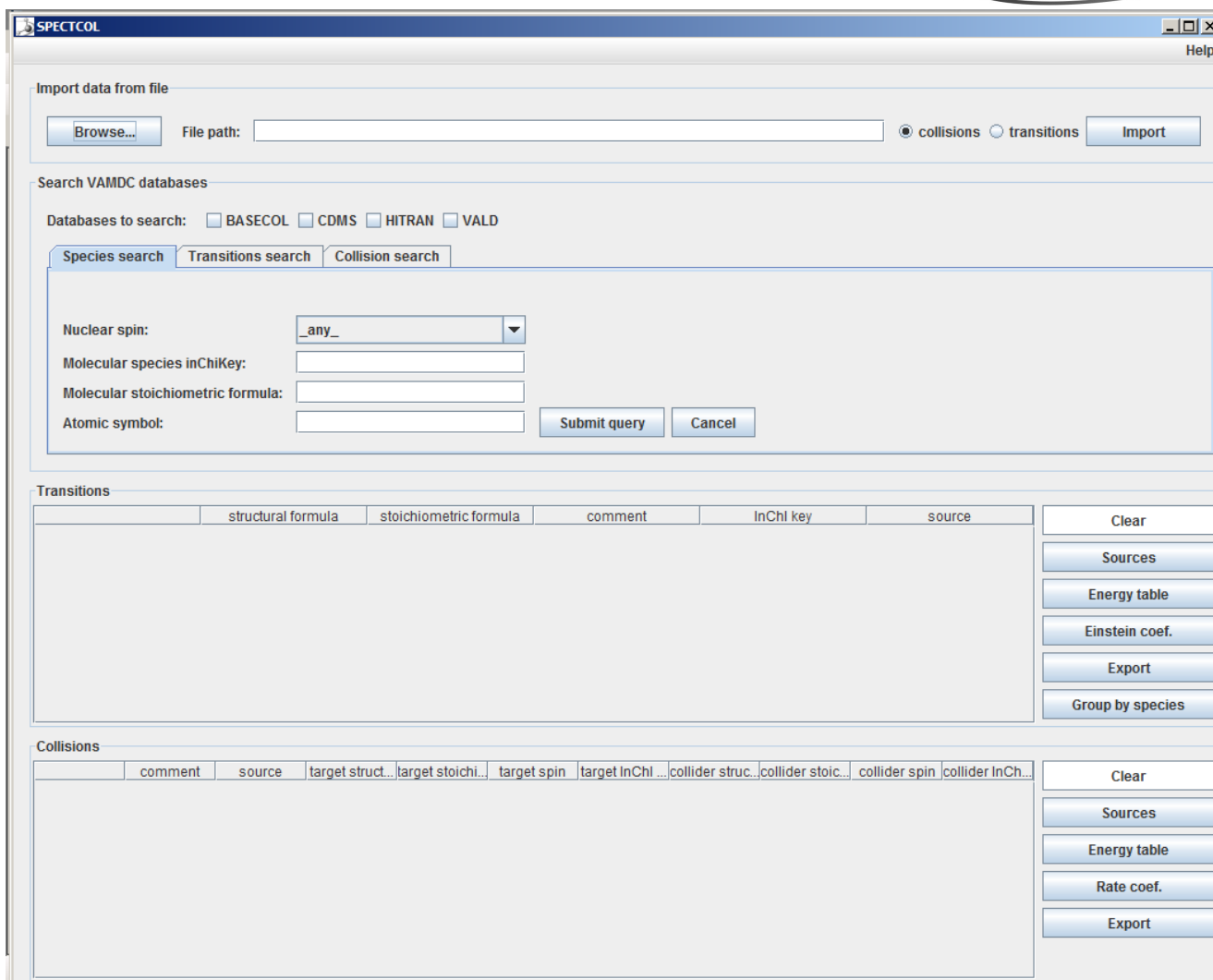
The `database.properties` file contains configuration properties necessary to connect to the registry and query the databases. It comes with pre-set default values but the advanced users can update these when needed. The properties are as follows:

- `registry.endpoint` – The URL of the registry endpoint
- `<DATABASENAME>.identifier` – the URL based identifier of the resource in the following form:
`ivo://{authorityid}/{resourcekey}`

For the values of registry keys for relevant databases consult the registry. For more information about registry identifiers visit <http://www.ivoa.net/Documents/REC/Identifiers/Identifiers-20070302.html>

The Main Panel

The main panel consists of four sections: import, search, transitions and collisions summary tables with control buttons.



The screenshot shows the SPECTCOL software interface. At the top right is the VAMDC logo. The main window has a title bar 'SPECTCOL' and a 'Help' button. Below the title bar is the 'Import data from file' section, which includes a 'Browse...' button, a 'File path:' text box, radio buttons for 'collisions' (selected) and 'transitions', and an 'Import' button. Below this is the 'Search VAMDC databases' section. It has checkboxes for 'BASECOL', 'CDMS', 'HITRAN', and 'VALD'. There are three tabs: 'Species search' (selected), 'Transitions search', and 'Collision search'. The 'Species search' tab contains a 'Nuclear spin:' dropdown menu (set to '_any_'), and three text input fields for 'Molecular species inChiKey:', 'Molecular stoichiometric formula:', and 'Atomic symbol:'. There are 'Submit query' and 'Cancel' buttons. Below the search section are two table views: 'Transitions' and 'Collisions'. Each table has a header row with columns for 'structural formula', 'stoichiometric formula', 'comment', 'InChI key', and 'source'. To the right of each table is a vertical stack of buttons: 'Clear', 'Sources', 'Energy table', 'Einstein coef.', 'Export', and 'Group by species' for transitions; and 'Clear', 'Sources', 'Energy table', 'Rate coef.', and 'Export' for collisions.

Import

Used for importing data from VAMDC-XSAMS files on hard drive.

Search

Used to search selected databases on the fly based on the few specific keywords.

The search consists of database selection check boxes and is divided into three tabs: Species, Transitions and Collisions. These correspond to different types of searches.

Species search tab

The species search is intended as a preview of species available in the databases. It will return only the species information, without any states and processes data. The search results will pop up in a new window shown below.

Species search result					
Species					
	structural formula	stoichiometric formula	comment	InChI key	source
1	Fe	Fe		XEEYBQQBJWHFJM-IGMARMGPSA	VALD 2011-09-02 00:43:32.689
2	Fe	Fe		WZGNVVUXVXNNOX-IGMARMGPSA	VALD 2011-09-02 00:43:32.689
3	Fe	Fe		CWYNVVG00AEACU-IGMARMGPSA	VALD 2011-09-02 00:43:32.689
4	Fe	Fe		VTLYFUHAOXGGBS-IGMARMGPSA	VALD 2011-09-02 00:43:32.689
5	Fe	Fe		SGGMZBKQLBLK-IGMARMGPSA	VALD 2011-09-02 00:43:32.689

Transitions search tab

The transitions search is used to search for radiative transitions. The results of this search are grouped by the transition's initial state species reference. If the data returned from the database contains no transitions, the results are grouped by the available species information. The summary of the results is displayed in the Transitions Summary table.

Collisions search tab

This tab is used to search for collisions. A target restriction is required and the collider restriction is optional. The results of this search are grouped by collision sets. If the data returned from the database contains no collisions, the results are grouped by the available species information. The summary of the results is displayed in the Collisions Summary table.

Note: *With every new search, the results will be appended to the data already loaded. The amount of data typically returned by these queries is very large. It is advised that the user occasionally clears the search results using the Clear button.*

Control buttons

The buttons available for both summary tables are:

- **Clear** – clears all data described in the summary table
- **Get sources** – displays in a table format the sources of data relevant to the selected molecule/atom from the summary table
- **Get energy table** – displays in a table format the energy levels and quantum numbers relevant to the selected molecule/atom from the summary table
- **Export** – makes a subset of the original data based on the molecule selected in the summary table and exports it as VAMDC-XSAMS formatted XML file, to a user specified location.

Transitions buttons:

- **Get Einstein coefficients** – displays in a table format the Einstein coefficients relevant to the selected molecule from the transitions summary table, if such data is available.

- **Group by species** – based on the selected molecule/atom in the transitions summary table groups all species from species with the same InChiKey and presents the information in a new panel from which the user can perform further data extraction and merging.

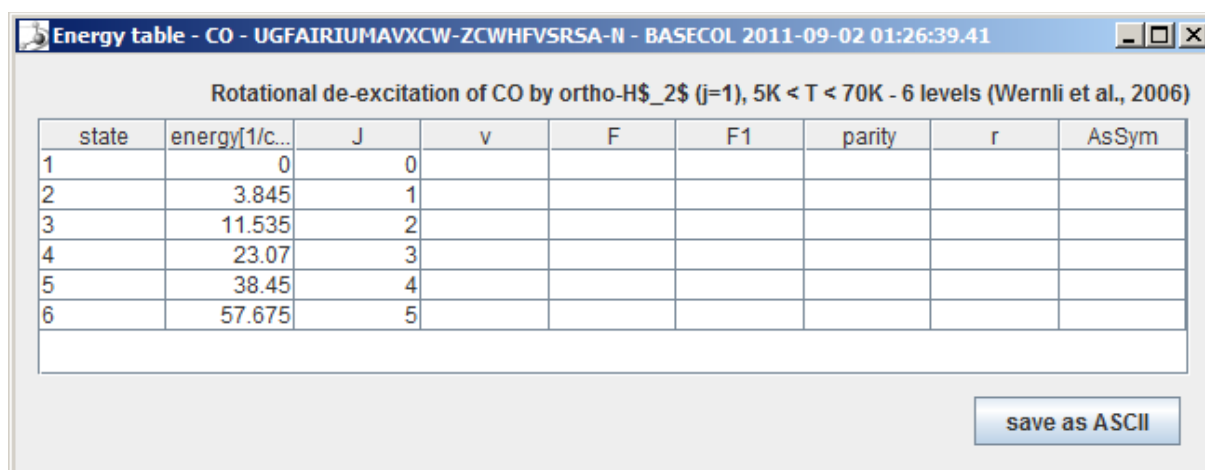
Collisions buttons:

- **Get rate coefficients** – displays in a table format the rate coefficients relevant to the selected collisions set from the collisions summary table, if such data is available.

Tabulated Data

Energy table

The energy table displays the state energy and quantum number information for the selected species. The quantum numbers available vary depending on the selected species. For definition of quantum numbers and more information on cases see the VAMDC-XSAMS documentation.



state	energy[1/c...	J	v	F	F1	parity	r	AsSym
1	0	0						
2	3.845	1						
3	11.535	2						
4	23.07	3						
5	38.45	4						
6	57.675	5						

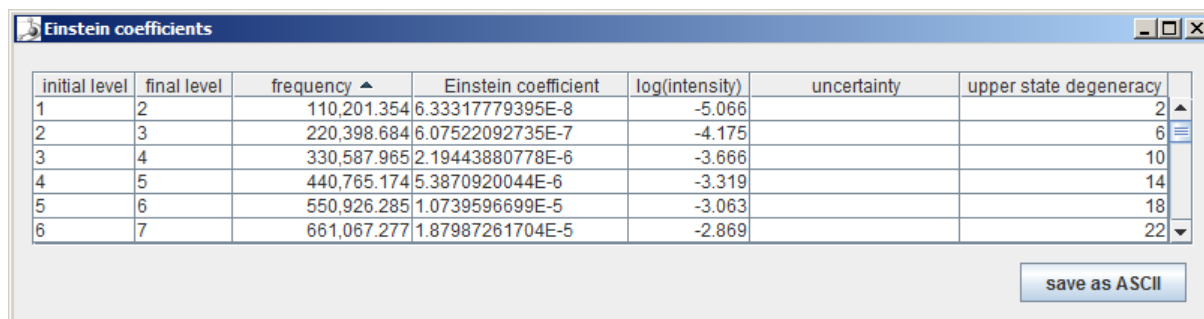
Einstein coefficients table

The Einstein coefficient data is displayed in the panel illustrated below. The columns of the table are:

- **initial level** – id of the initial state of a radiative transition. It can be used to identify the energy and quantum numbers from the energy table.
- **final level** – id of the final state of a radiative transition. It can be used to identify the energy and quantum numbers from the energy table.
- **frequency**
- Einstein coefficient
- **log(Intensity)**

- **uncertainty**
- **upper state degeneracy**

This information can be exported into a text file with comma separated values by clicking the "Save as ASCII" button.

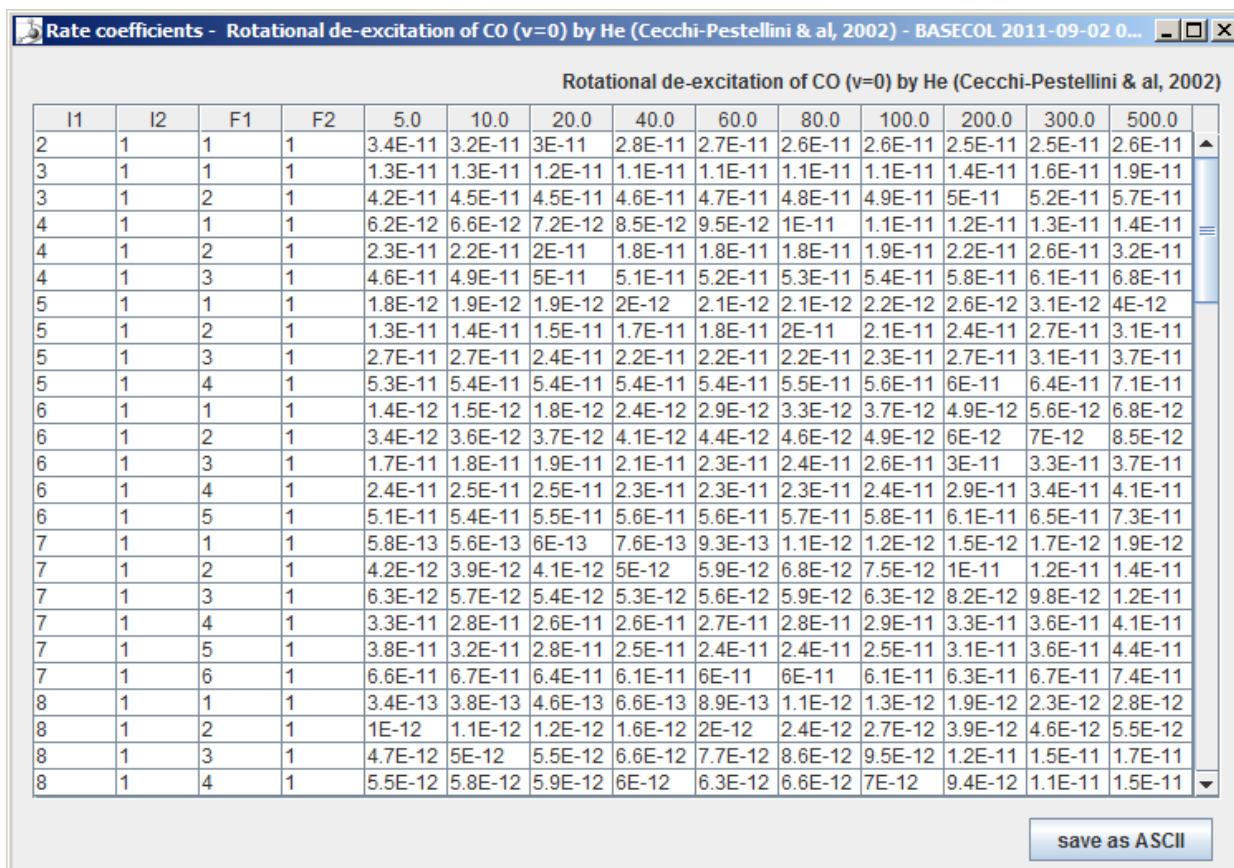


initial level	final level	frequency \uparrow	Einstein coefficient	log(intensity)	uncertainty	upper state degeneracy
1	2	110,201.354	6.33317779395E-8	-5.066		2
2	3	220,398.684	6.07522092735E-7	-4.175		6
3	4	330,587.965	2.19443880778E-6	-3.666		10
4	5	440,765.174	5.3870920044E-6	-3.319		14
5	6	550,926.285	1.0739596699E-5	-3.063		18
6	7	661,067.277	1.87987261704E-5	-2.869		22

Rate coefficients table

The rate coefficient data is displayed in the panel illustrated below.

This information can be exported into a text file with comma separated values by clicking the "Save as ASCII" button.



Rotational de-excitation of CO (v=0) by He (Cecchi-Pestellini & al, 2002)													
I1	I2	F1	F2	5.0	10.0	20.0	40.0	60.0	80.0	100.0	200.0	300.0	500.0
2	1	1	1	3.4E-11	3.2E-11	3E-11	2.8E-11	2.7E-11	2.6E-11	2.6E-11	2.5E-11	2.5E-11	2.6E-11
3	1	1	1	1.3E-11	1.3E-11	1.2E-11	1.1E-11	1.1E-11	1.1E-11	1.1E-11	1.4E-11	1.6E-11	1.9E-11
3	1	2	1	4.2E-11	4.5E-11	4.5E-11	4.6E-11	4.7E-11	4.8E-11	4.9E-11	5E-11	5.2E-11	5.7E-11
4	1	1	1	6.2E-12	6.6E-12	7.2E-12	8.5E-12	9.5E-12	1E-11	1.1E-11	1.2E-11	1.3E-11	1.4E-11
4	1	2	1	2.3E-11	2.2E-11	2E-11	1.8E-11	1.8E-11	1.8E-11	1.9E-11	2.2E-11	2.6E-11	3.2E-11
4	1	3	1	4.6E-11	4.9E-11	5E-11	5.1E-11	5.2E-11	5.3E-11	5.4E-11	5.8E-11	6.1E-11	6.8E-11
5	1	1	1	1.8E-12	1.9E-12	1.9E-12	2E-12	2.1E-12	2.1E-12	2.2E-12	2.6E-12	3.1E-12	4E-12
5	1	2	1	1.3E-11	1.4E-11	1.5E-11	1.7E-11	1.8E-11	2E-11	2.1E-11	2.4E-11	2.7E-11	3.1E-11
5	1	3	1	2.7E-11	2.7E-11	2.4E-11	2.2E-11	2.2E-11	2.2E-11	2.3E-11	2.7E-11	3.1E-11	3.7E-11
5	1	4	1	5.3E-11	5.4E-11	5.4E-11	5.4E-11	5.4E-11	5.5E-11	5.6E-11	6E-11	6.4E-11	7.1E-11
6	1	1	1	1.4E-12	1.5E-12	1.8E-12	2.4E-12	2.9E-12	3.3E-12	3.7E-12	4.9E-12	5.6E-12	6.8E-12
6	1	2	1	3.4E-12	3.6E-12	3.7E-12	4.1E-12	4.4E-12	4.6E-12	4.9E-12	6E-12	7E-12	8.5E-12
6	1	3	1	1.7E-11	1.8E-11	1.9E-11	2.1E-11	2.3E-11	2.4E-11	2.6E-11	3E-11	3.3E-11	3.7E-11
6	1	4	1	2.4E-11	2.5E-11	2.5E-11	2.3E-11	2.3E-11	2.3E-11	2.4E-11	2.9E-11	3.4E-11	4.1E-11
6	1	5	1	5.1E-11	5.4E-11	5.5E-11	5.6E-11	5.6E-11	5.7E-11	5.8E-11	6.1E-11	6.5E-11	7.3E-11
7	1	1	1	5.8E-13	5.6E-13	6E-13	7.6E-13	9.3E-13	1.1E-12	1.2E-12	1.5E-12	1.7E-12	1.9E-12
7	1	2	1	4.2E-12	3.9E-12	4.1E-12	5E-12	5.9E-12	6.8E-12	7.5E-12	1E-11	1.2E-11	1.4E-11
7	1	3	1	6.3E-12	5.7E-12	5.4E-12	5.3E-12	5.6E-12	5.9E-12	6.3E-12	8.2E-12	9.8E-12	1.2E-11
7	1	4	1	3.3E-11	2.8E-11	2.6E-11	2.6E-11	2.7E-11	2.8E-11	2.9E-11	3.3E-11	3.6E-11	4.1E-11
7	1	5	1	3.8E-11	3.2E-11	2.8E-11	2.5E-11	2.4E-11	2.4E-11	2.5E-11	3.1E-11	3.6E-11	4.4E-11
7	1	6	1	6.6E-11	6.7E-11	6.4E-11	6.1E-11	6E-11	6E-11	6.1E-11	6.3E-11	6.7E-11	7.4E-11
8	1	1	1	3.4E-13	3.8E-13	4.6E-13	6.6E-13	8.9E-13	1.1E-12	1.3E-12	1.9E-12	2.3E-12	2.8E-12
8	1	2	1	1E-12	1.1E-12	1.2E-12	1.6E-12	2E-12	2.4E-12	2.7E-12	3.9E-12	4.6E-12	5.5E-12
8	1	3	1	4.7E-12	5E-12	5.5E-12	6.6E-12	7.7E-12	8.6E-12	9.5E-12	1.2E-11	1.5E-11	1.7E-11
8	1	4	1	5.5E-12	5.8E-12	5.9E-12	6E-12	6.3E-12	6.6E-12	7E-12	9.4E-12	1.1E-11	1.5E-11

Importing existing VAMDC-XSAMS files

The application allows the user to import files already saved on their computer. The files must be correctly formatted XML files which conform to the VAMDC-XSAMS standard. For the more information about the VAMDC-XSAMS standard see <http://www.vamdc.org/documents/standards/> .

To import an existing file:

1. click the "Browse" button
2. select the file of interest
3. select "transitions" or "collisions" to specify how to treat the imported data
4. click "Open". This will fill the file path information.
5. click the "Import" button

Alternatively you can type the file path information manually.

Searching VAMDC databases

The application can be used to search selected VAMDC databases directly.

1. Select the databases to search by selecting the appropriate check boxes. Selecting a database will automatically disable the keyword options not available for the selected database. If several databases are selected only the keywords which can be used for all selected databases are available.
2. Fill in one of the keyword values for your search. If several fields are filled in only the topmost keyword will be used for the search.
3. Click "Submit Query". Search results will appear in the summary table

Grouping data

By selecting a row in the Transitions Summary table you identify the species you wish to use as a reference for data grouping. Clicking the "Group species" button groups the loaded data based on the selected species' inChiKey. For transitions this means all the information concerning species with the same inChiKey. For collisions, this implies that the target element involved in the collision has the same inChiKey.

This is the first step in identifying what data can be merged. The selection is displayed in the Group Panel, shown below.

Species inChiKey: UGFAIRIUMAVXCW-ZCWHFVSRSA-N

Select a row from each table

Transitions

	structural formula	stoichiometric formula	comment	InChI key	source
1	CO	CO		UGFAIRIUMAVXCW-Z...	CDMS 2011-09-03 23...
2	CO	CO		UGFAIRIUMAVXCW-Z...	CDMS 2011-09-03 23...

Collisions

	comment	source	target struct...	target stoic...	target spin	target InChI...	collider stru...	collider stoi...	collider spin	collider InC...
1	Rotational ...	BASECOL ...	CO	CO		UGFAIRIU...	H\$_2\$	H2	para	UFHFLCQ...
2	Rotational ...	BASECOL ...	CO	CO		UGFAIRIU...	H\$_2\$	H2	ortho	UFHFLCQ...
3	Rotational ...	BASECOL ...	CO	CO		UGFAIRIU...	H\$_2\$	H2	para	UFHFLCQ...
4	Rotational...	BASECOL ...	CO	CO		UGFAIRIU...	H	H		YZCKVEUI...
5	Vibrational ...	BASECOL ...	CO	CO		UGFAIRIU...	H	H		YZCKVEUI...
6	Rotational...	BASECOL ...	CO	CO		UGFAIRIU...	He	He		SWQJXJO...
7	Vibrational ...	BASECOL ...	CO	CO		UGFAIRIU...	He	He		SWQJXJO...
8	Rotational...	BASECOL ...	CO	CO		UGFAIRIU...	H	H		YZCKVEUI...
9	Rotational ...	BASECOL ...	CO	CO		UGFAIRIU...	H\$_2\$	H2	ortho	UFHFLCQ...
10	Rotational ...	BASECOL ...	CO	CO		UGFAIRIU...	H\$_2\$	H2	para	UFHFLCQ...
11	Rotational ...	BASECOL ...	CO	CO		UGFAIRIU...	H\$_2\$	H2	ortho	UFHFLCQ...

Show selection Export as XSAMS

By selecting a row from each table, the user identifies two sets of data they wish to merge. The data can either be exported straight to disc, in VAMDC-XSAMS format, or viewed in the GUI.

The merge is performed in the following way:

- the selection from the transitions table identifies the energy states
- for all the collisions in the selected collisions set, we replace the *target* state reference from the original data, with the equivalent state from the transition data
- two states are considered the same if they contain the same quantum numbers values
- if we can not find the equivalent state in the transition data, we drop the collision from the merge
- the state values of the collider elements remain the same
- all related source, method and function references are also added to the new data

The merged data can be displayed in a panel shown below.

State energy and quantum numbers								
state	energy[1/cm]	J	v	F	F1	parity	r	AsSym
1	0	0	0					
2	3.845	1	0					
3	11.535	2	0					
4	23.069	3	0					
5	38.448	4	0					
6	57.67	5	0					
7	80.735	6	0					
8	107.642	7	0					
9	138.39	8	0					
10	172.978	9	0					
11	211.404	10	0					

Rate coefficients													
I1	I2	F1	F2	100.0	200.0	300.0	500.0	700.0	1000.0	1500.0	2000.0	2500.0	3000.0
2	1	1	1	2.37E-10	2.47E-10	2.48E-10	2.44E-10	2.38E-10	2.31E-10	2.18E-10	2.05E-10	1.91E-10	1.77E-10
3	1	1	1	7.19E-11	7.59E-11	8.14E-11	9.54E-11	1.1E-10	1.29E-10	1.51E-10	1.62E-10	1.64E-10	1.61E-10
3	1	2	1	3.18E-10	3.29E-10	3.32E-10	3.3E-10	3.26E-10	3.2E-10	3.07E-10	2.91E-10	2.73E-10	2.55E-10
4	1	1	1	1.47E-11	1.67E-11	1.86E-11	2.11E-11	2.24E-11	2.3E-11	2.16E-11	1.92E-11	1.69E-11	1.48E-11
4	1	2	1	1.23E-10	1.31E-10	1.43E-10	1.69E-10	1.93E-10	2.22E-10	2.52E-10	2.65E-10	2.65E-10	2.59E-10
4	1	3	1	3.52E-10	3.57E-10	3.57E-10	3.54E-10	3.49E-10	3.41E-10	3.28E-10	3.12E-10	2.94E-10	2.75E-10
5	1	1	1	2.07E-11	2.19E-11	2.42E-11	2.81E-11	3.06E-11	3.26E-11	3.38E-11	3.34E-11	3.22E-11	3.05E-11
5	1	2	1	3.81E-11	3.81E-11	3.91E-11	4.06E-11	4.16E-11	4.31E-11	4.52E-11	4.59E-11	4.53E-11	4.38E-11
5	1	3	1	1.4E-10	1.51E-10	1.65E-10	1.93E-10	2.18E-10	2.49E-10	2.81E-10	2.95E-10	2.95E-10	2.88E-10
5	1	4	1	3.6E-10	3.66E-10	3.67E-10	3.63E-10	3.57E-10	3.49E-10	3.36E-10	3.2E-10	3.02E-10	2.82E-10
6	1	1	1	9.62E-12	8.38E-12	7.84E-12	7.05E-12	6.6E-12	6.42E-12	6.76E-12	7.15E-12	7.32E-12	7.29E-12

Einstein coefficients						
initial level	final level	frequency	Einstein coefficient	log(intensity)	uncertainty	upper state degen...
1	2	115,271.202	7.20378864479E-8	-5.01		1
2	3	230,538	6.91079000503E-7	-4.12		3
3	4	345,795.99	2.49670085538E-6	-3.612		5
4	5	461,040.768	6.12668117242E-6	-3.266		7
5	6	576,267.931	1.22134274135E-5	-3.012		9
6	7	691,473.076	2.13750692698E-5	-2.819		11
7	8	806,651.801	3.42239824576E-5	-2.672		13
8	9	921,799.704	5.13419191151E-5	-2.559		15
9	10	1,036,912.385	7.33007011041E-5	-2.475		17
10	11	1,151,985.443	1.00638923207E-4	-2.416		19
11	12	1,267,014.482	1.33903406762E-4	-2.377		21

Collider state energy and quantum numbers												
state	energy[1/cm]	parity	J	F	M	Kappa	term type	l	S	j	S2	K
1	0		0				LS	0	0			