

SPECTCOL improved with VO- Table and SAMP support

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SPECTCOL

- A graphical tool (Swing) implemented in Java.
- Manipulates and combines spectroscopic and collisional data coming from the Databases (CDMS, JPL, BASECOL, HITRAN,...) using VAMDC technology.
- Manipulates and provides methods to convert XSAMS(Xml Schema for Atoms, Molecules and Solids) data into other formats (CSV, RADEX, LTE).

<http://www.vamdc.org/activities/research/software/spectcol/>

SPECTCOL main panel

Import Panel

Search Panel

Spectroscopic data results

Collisional data results

Buttons to Manipulate data

The screenshot displays the SPECTCOL main panel, which is divided into several functional areas:

- Import Panel:** Located at the top, it includes a "Browse..." button for file selection, a "File path:" input field, radio buttons for "collisions", "transitions", and "Merged data by Spectcol", and an "Import" button.
- Search Panel:** Below the import section, it features a "Search VAMDC databases" area with a "Select databases" button. It has two tabs: "Species search" and "Transitions & Collisions search". The "Transitions & Collisions search" tab is active, showing a search form with fields for "Nuclear spin:" (set to "_any_"), "Molecular species InChiKey:", "Molecular stoichiometric formula:" (set to "CO"), "Ion charge:", "Atomic symbol:", and "Particle name:". "Submit query" and "Cancel" buttons are at the bottom of the form.
- Transitions Table:** A table with columns: comment, source, structural formula, stoichiometric formula, spin, and InChi key. It lists 7 transition entries.
- Collisional Table:** A table with columns: comment, source, target structu..., target stoichi..., target spin, target InChi key, collider structu..., collider stoich..., collider spin, and collider InChi... It lists 11 collisional entries.
- Manipulation Buttons:** On the right side of each table, there are buttons for "Clear", "Sources", "Energy table", "Einstein coef.", "Partition func.", "Export", "Group by hand", and "Group by species".

SPECTCOL : Interoperability

Spectcol can send data table with SAMP (which was easily integrated)

- Data are sent in VO-Table format
- All tables (Energies, Einstein coefficients, Rate coefficients and Partition functions) can be sent to any tool accepting VO-Table such as TopCat

Use case (1): Plot CO Einstein Coeff. with TopCat

1. Select a database (ex : CDMS)

The screenshot shows the SPECTCOL software interface. At the top, there is a title bar with 'SPECTCOL' and 'Policy Citation Help'. Below this, there are sections for 'Import data from file' and 'Search VAMDC databases'. The 'Search VAMDC databases' section is active, showing a 'Select databases' button. Below this, there are search criteria fields for 'Processes' (Collisions, Transitions, Collisions & Transitions) and 'Form' (Nuclear spin, Molecular species InChIKey, Molecular stoichiometric formula, Ion charge, Atomic symbol, Particle name). There are also 'Submit query' and 'Cancel' buttons. At the bottom, there are sections for 'Transitions' and 'Collisions' with various search criteria and buttons like 'Clear', 'Sources', 'Energy table', 'Einstein coef.', 'Partition func.', 'Export', 'Group by hand', and 'Group by species'.

The screenshot shows the 'Databases' window with a table of databases. The 'CDMS' database is selected, indicated by a checkmark in the 'Selected' column. The table has columns for Title, Description, Status, Selected, and Ivoid.

Title	Description	Status	Selected	Ivoid
Belgrade el...	Electron int...	active	<input type="checkbox"/>	ivo://vamdc/...
TFMeCaSDa...	Calculated l...	active	<input type="checkbox"/>	ivo://vamdc/...
Photodisso...	Database f...	active	<input type="checkbox"/>	ivo://vamdc/...
Chianti	Chianti con...	active	<input type="checkbox"/>	ivo://vamdc/...
GSMA Reim...	Calculated l...	active	<input type="checkbox"/>	ivo://vamdc/...
ECaSDa - Et...	Calculated ...	active	<input type="checkbox"/>	ivo://vamdc/...
GhoSST	The GhoSST...	active	<input type="checkbox"/>	ivo://vamdc/...
SHeCaSDa - ...	Calculated l...	active	<input type="checkbox"/>	ivo://vamdc/...
Stark-b	Database f...	active	<input type="checkbox"/>	ivo://vamdc/...
JPL databas...	The JPL dat...	active	<input type="checkbox"/>	ivo://vamdc/...
HITRANonline	The HITRAN ...	active	<input type="checkbox"/>	ivo://vamdc/...
VALD sub-s...	The part of ...	active	<input type="checkbox"/>	ivo://vamdc/...
RADAM - Ion...	Database f...	active	<input type="checkbox"/>	ivo://vamdc/...
MeCaSDa - ...	Calculated l...	active	<input type="checkbox"/>	ivo://vamdc/...
VALD (atoms)	The Vienna ...	active	<input type="checkbox"/>	ivo://vamdc/...
VAMDC spe...	This Databa...	active	<input type="checkbox"/>	ivo://vamdc/...
LXcat	An open-ac...	active	<input type="checkbox"/>	ivo://vamdc/...
OACT - LASP...	Laboratori...	active	<input type="checkbox"/>	ivo://vamdc/...
TOPbase : V...	TOPbase lis...	active	<input type="checkbox"/>	ivo://vamdc/...
BASECOL: V...	This databa...	active	<input type="checkbox"/>	ivo://vamdc/...
UMIST Data...	Reaction ra...	active	<input type="checkbox"/>	ivo://vamdc/...
IDEADB - In...	This databa...	active	<input type="checkbox"/>	ivo://vamdc/...
TIPbase : V...	TIPbase list...	active	<input type="checkbox"/>	ivo://vamdc/...
CDMS	The Cologn...	active	<input checked="" type="checkbox"/>	ivo://vamdc/...
Carbon Diox...	Carbon Diox...	active	<input type="checkbox"/>	ivo://vamdc/...

Use case (1): Plot CO Einstein Coeff. with TopCat

2. Select the transition process and Search a molecule (ex : CO)

The SPECTCOL interface shows search criteria for transitions. The 'Processes' section has 'Transitions' selected. The 'Form' section includes 'Nuclear spin' set to '_any_', 'Molecular species InChIKey' and 'Molecular stoichiometric formula' both set to 'CO'. The 'Upper state energy' and 'Lower state energy' are both set to '1/cm'. The 'Probability, A' field is empty. A table of transitions is displayed below, with the third entry selected.

	comment	source	structural formula	stoichiometric formula	spin	InChI key
1	30502-v1:CO-18; \$v=0\$	CDMS 2015-06-09 18...	CO-18	CO		UGFAIRIUMAVXCW-HQ...
2	29501-v2*:C13-0; \$v=0\$	CDMS 2015-06-09 18...	C-13-0	CO		UGFAIRIUMAVXCW-OU...
3	28503-v1:CO; \$v=0\$	CDMS 2015-06-09 18...	CO	CO		UGFAIRIUMAVXCW-UH...
4	29503-v1:CO-17; \$v=0\$	CDMS 2015-06-09 18...	CO-17	CO		UGFAIRIUMAVXCW-VQ...
5	31502-v1:C13-0-18; \$v=0\$	CDMS 2015-06-09 18...	C-13-0-18	CO		UGFAIRIUMAVXCW-RG...
6	28512-v1*:CO; \$v=1,2,3\$	CDMS 2015-06-09 18...	CO	CO		UGFAIRIUMAVXCW-UH...
7	30503-v1:C13-0-17; \$v=0\$	CDMS 2015-06-09 18...	C-13-0-17	CO		UGFAIRIUMAVXCW-ZD...

3. Select a sepectroscopic dataset

4. Display Einstein table

The 'Einstein coefficients' window displays a table for the dataset '28503-v 1:CO; \$v=0\$'. The table has columns for upper level, lower level, frequency, Einstein coefficient, log(intensity), uncertainty, and upper level. The 'Einstein coef.' column is highlighted. Buttons for 'Send by SAMP' and 'save as ASCII' are at the bottom.

uppe...	lower le...	frequen...	Einstein...	log(inte...	uncerta...	upper d...
2	1	115271...	7.2036...	-5.0105	5.0E-4	3
3	2	230538.0	6.9106...	-4.1197	5.0E-4	5
4	3	345795...	2.4966...	-3.6118	5.0E-4	7
5	4	461040...	6.1265...	-3.2657	5.0E-4	9
6	5	576267...	1.2213...	-3.0118	5.0E-4	11
7	6	691473...	2.1374...	-2.8193	5.0E-4	13
8	7	806651...	3.4223...	-2.6716	0.005	15
9	8	921799.7	5.1340...	-2.559	0.005	17
10	9	103691...	7.3298...	-2.4751	0.005	19
11	10	115198...	1.0063...	-2.4156	0.011	21
12	11	126701...	1.3389...	-2.3773	0.005	23
13	12	138199...	1.7352...	-2.3581	0.013	25
14	13	149692...	2.2003...	-2.3561	0.012	27
15	14	161179...	2.7389...	-2.3699	0.011	29
16	15	172660...	3.3534...	-2.3987	0.0024	31
17	16	184134...	4.0498...	-2.4413	0.011	33
18	17	195601...	4.8286...	-2.4973	0.011	35
19	18	207061...	5.6948...	-2.5659	0.014	37
20	19	218513...	6.6496...	-2.6467	0.013	39
21	20	229956...	7.6947...	-2.7393	0.01	41
22	21	241391...	8.8322...	-2.8433	0.011	43
23	22	252817...	0.0010...	-2.9584	0.011	45
24	23	264233...	0.0011...	-3.0843	0.0039	47
25	24	275638...	0.0012...	-3.2209	0.017	49
26	25	287033...	0.0014...	-3.3678	0.013	51

Use case (1): Plot CO Einstein Coeff. with TopCat

upper...	lower le...	frequen...	Einstein...	log(inte...	uncerta...	upper d...
2	1	115271...	7.2036...	-5.0105	5.0E-4	3
3	2	230538.0	6.9106...	-4.1197	5.0E-4	5
4	3	345795...	2.4966...	-3.6118	5.0E-4	7
5	4	461040...	6.1265...	-3.2657	5.0E-4	9
6	5	576267...	1.2213...	-3.0118	5.0E-4	11
7	6	691473...	2.1374...	-2.8193	5.0E-4	13
8	7	806651...	3.4223...	-2.6716	0.005	15
9	8	921799.7	5.1340...	-2.559	0.005	17
10	9	103691...	7.3298...	-2.4751	0.005	19
11	10	115198...	1.0063...	-2.4156	0.011	21
12	11	126701...	1.3389...	-2.3773	0.005	23
13	12	138199...	1.7352...	-2.3581	0.013	25
14	13	149692...	2.2003...	-2.3561	0.012	27
15	14	161179...	2.7389...	-2.3699	0.011	29
16	15	172660...	3.3534...	-2.3987	0.0024	31
17	16	184134...	4.0498...	-2.4413	0.011	33
18	17	195601...	4.8286...	-2.4973	0.011	35
19	18	207061...	5.6948...	-2.5659	0.014	37
20	19	218513...	6.6496...	-2.6467	0.013	39
21	20	229956...	7.6947...	-2.7393	0.01	41
22	21	241391...	8.8322...	-2.8433	0.011	43
23	22	252817...	0.0010...	-2.9584	0.011	45
24	23	264233...	0.0011...	-3.0843	0.0039	47
25	24	275638...	0.0012...	-3.2209	0.017	49
26	25	287033...	0.0014...	-3.3678	0.013	51

5. Launch TopCat first and send it Einstein table

TOPCAT

File Views Graphics Joins Windows VO Interop Help

Table List

- 1: Sp_CO Einstein

Current Table Properties

- Label: Sp_CO Einstein
- Location: Spectcol:Sp_CO Einstein
- Name: Sp_CO Einstein
- Rows: 95
- Columns: 8
- Sort Order: ↑
- Row Subset: All
- Activation Action: (no action) Broadcast Row

SAMP

Messages: Clients:

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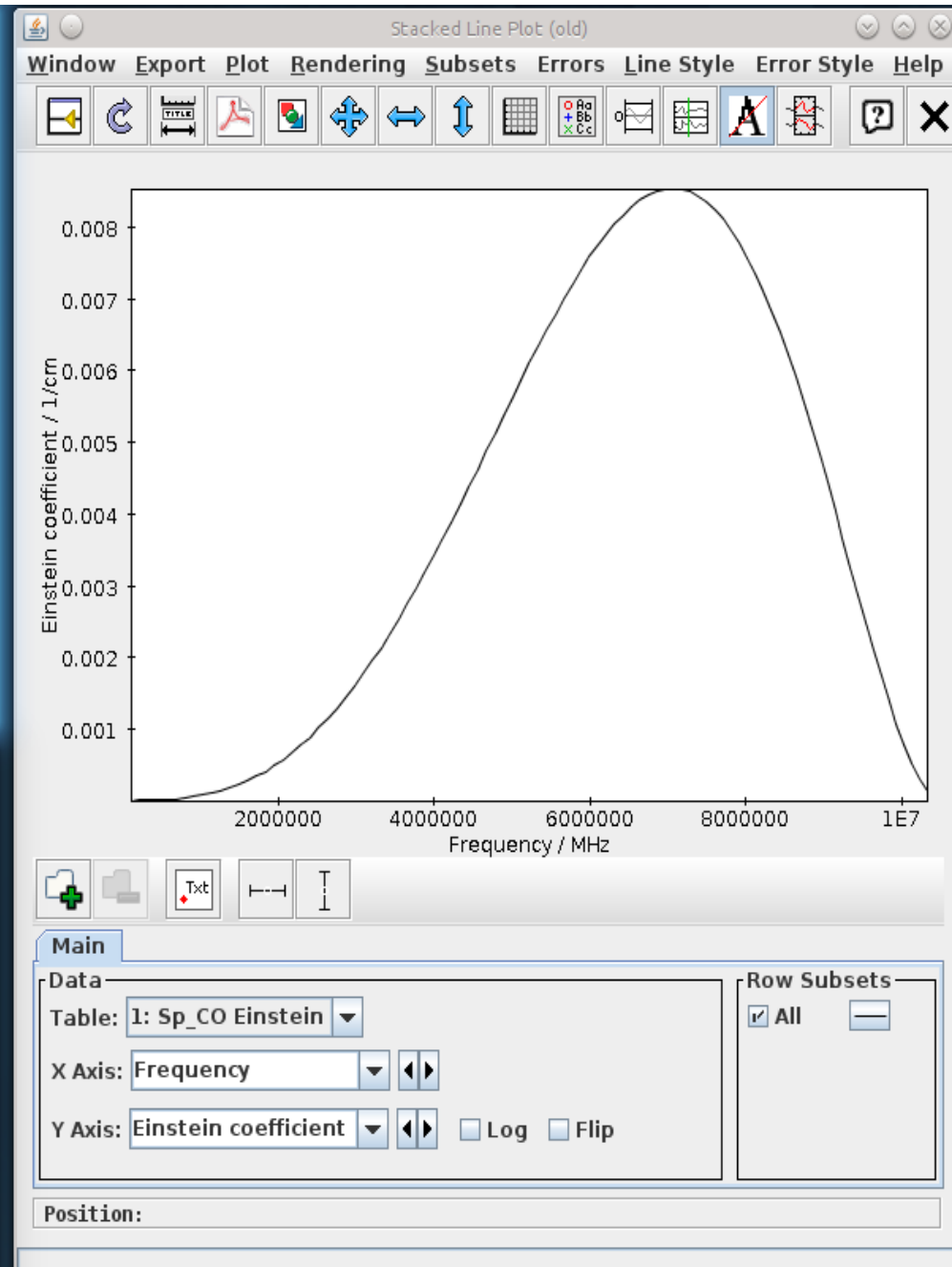
Use case (1) : Plot CO Einstein Coeff. with TopCat

TOPCAT(1): Table Browser

Window Subsets Help

Table Browser for 1: Sp_CO Einstein

	Index	Upper ...	Lower l...	Frequency	Einstein coeff...	log(intensi...	Uncertainty	Upper ...
1	1	2	1	1,152712E5	7,203603E-8	-5,0105	0,0005	3
2	2	3	2	2,305380E5	6,910612E-7	-4,1197	0,0005	5
3	3	4	3	3,457960E5	2,496637E-6	-3,6118	0,0005	7
4	4	5	4	4,610408E5	6,126524E-6	-3,2657	0,0005	9
5	5	6	5	5,762679E5	1,221311E-5	-3,0118	0,0005	11
6	6	7	6	6,914731E5	2,137452E-5	-2,8193	0,0005	13
7	7	8	7	8,066518E5	3,422310E-5	-2,6716	0,005	15
8	8	9	8	9,217997E5	5,134060E-5	-2,559	0,005	17
9	9	10	9	1,036912E6	7,329882E-5	-2,4751	0,005	19
10	10	11	10	1,151985E6	0,0001	-2,4156	0,011	21
11	11	12	11	1,267014E6	0,00013	-2,3773	0,005	23
12	12	13	12	1,381995E6	0,00017	-2,3581	0,013	25
13	13	14	13	1,496923E6	0,00022	-2,3561	0,012	27
14	14	15	14	1,611794E6	0,00027	-2,3699	0,011	29
15	15	16	15	1,726603E6	0,00034	-2,3987	0,0024	31
16	16	17	16	1,841346E6	0,0004	-2,4413	0,011	33
17	17	18	17	1,956089E6	0,00048	-2,4872	0,011	35



TOPCAT

File Views Graphics Joins Windows VO Interop Help

Table List

1: Sp_CO Einstein

Current Table Properties

Label: Sp_CO Einstein

Location: Spectcol:Sp_CO Einstein

Name: Sp_CO Einstein

Rows: 95

Columns: 8

Sort Order: ↑

Row Subset: All

SAMP

Messages: ○ Clients:

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Use case (2) : Plot CO-HE Rate Coeff. with TopCat

2 options to send data by SAMP :

- Visualize all transitions for each temperature
- Visualize all the temperatures for one transition

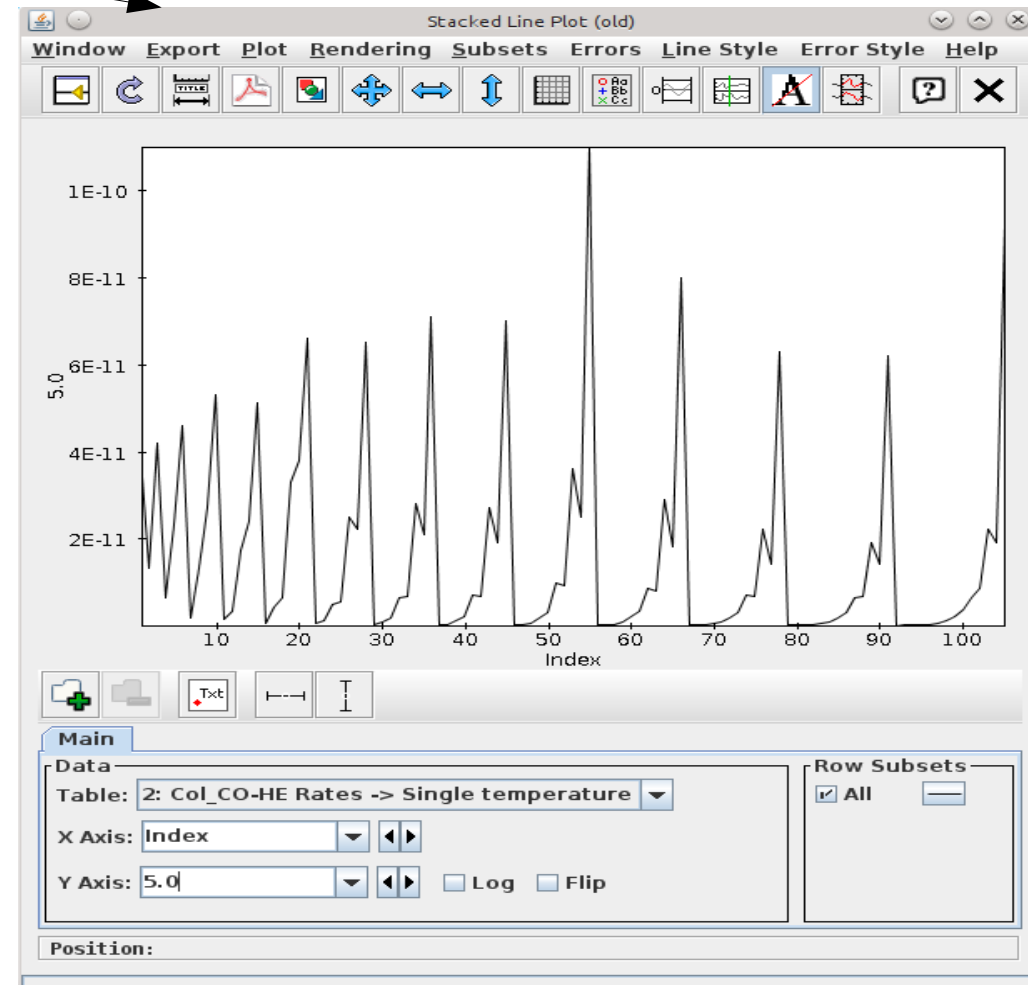
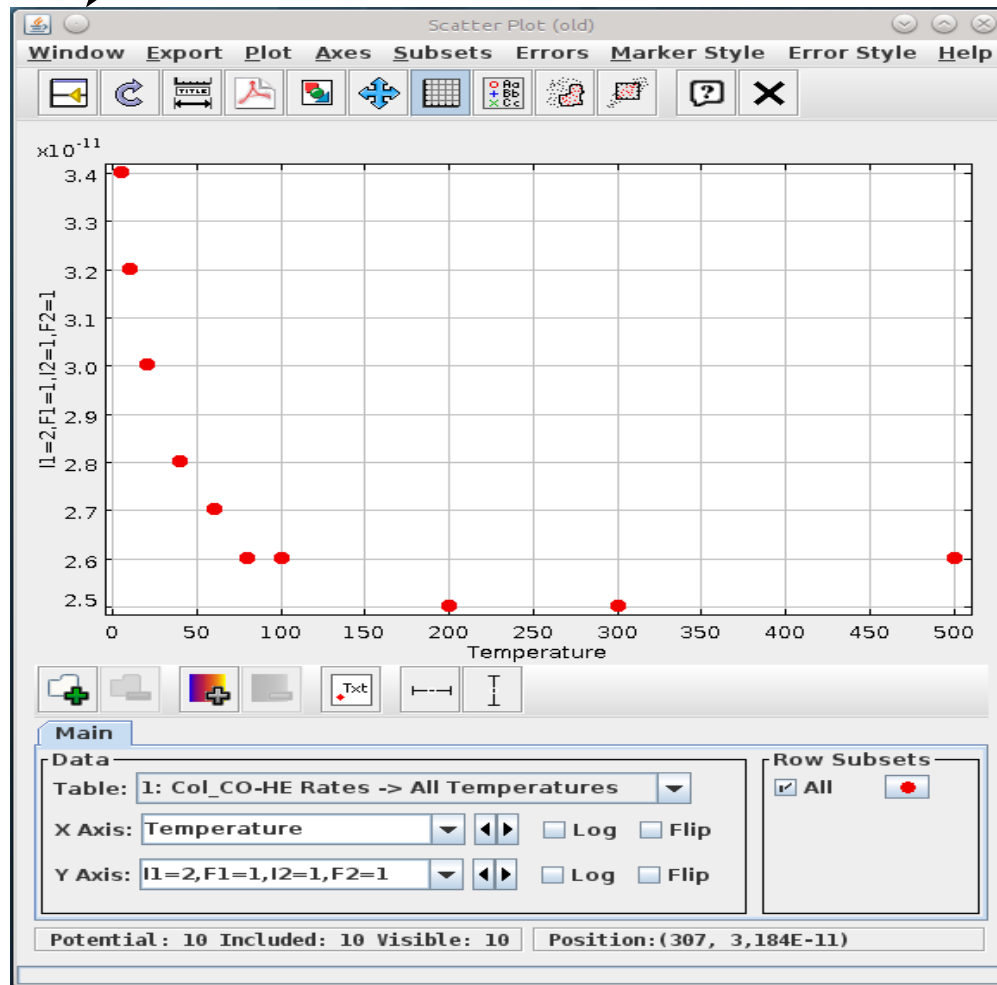
The screenshot shows a software window titled "Rate coefficients - Rotational de-excitation of CO (v=0) by He (Cecc...)" with a subtitle "Rotational de-excitation of CO (v=0) by He (Cecchi-Pestellini & al, 2002)". The window contains a table with columns labeled J1, F1, J2, F2, and various temperature values (5.0, 10.0, 20.0, 40.0, 60.0, 80.0, 10..., 20..., 30..., 50...). A dialog box titled "Select Format" is overlaid on the table, asking the user to "Select the format you want to send to TopCat". The dialog box has three options: "All temperatures", "All temperatures", and "One by one temperature". At the bottom of the window, there are two buttons: "Send by SAMP" and "save as ASCII".

J1	F1	J2	F2	5.0	10.0	20.0	40.0	60.0	80.0	10...	20...	30...	50...
2	1	1	1	3.4...	3...	3E...	2...	2.7...	2...	2.6...	2...	2.5...	2...
3	1	1	1	1.3...	1...	1.2...	1...	1.1...	1...	1.1...	1...	1.6...	1...
3	2	1	1	4.2...	4...	4.5...	4...	4.7...	4...	4.9...	5E...	5.2...	5...
4	1	1	1	6.2...	6...	7.2...	8...	9.5...	1E...	1.1...	1...	1.3...	1...
4	2	1	1	2.3...	2...	2E...	1...	1.8...	1...	1.9...	2...	2.6...	3...
4	3	1	1	4.6...	4...	5E...	5...	5.2...	5...	5.4...	5...	6.1...	6...
5	1	1	1	1.8...	1...	1.9...	2E...	2.1...	2...	2.2...	2...	3.1...	4E...
5	2											7...	3...
5	3											1...	3...
5	4											4...	7...
6	1											6...	6...
6	2											5...	8...
6	3											3...	3...
6	4											4...	4...
6	5											5...	7...
7	1	1	1	5.8...	5...	6E...	7...	9.3...	1...	1.2...	1...	1.7...	1...
7	2	1	1	4.2...	3...	4.1...	5E...	5.9...	6...	7.5...	1E...	1.2...	1...
7	3	1	1	6.3...	5...	5.4...	5...	5.6...	5...	6.3...	8...	9.8...	1...
7	4	1	1	3.3...	2...	2.6...	2...	2.7...	2...	2.9...	3...	3.6...	4...
7	5	1	1	3.8...	3...	2.8...	2...	2.4...	2...	2.5...	3...	3.6...	4...
7	6	1	1	6.6...	6...	6.4...	6...	6E...	6E...	6.1...	6...	6.7...	7...
8	1	1	1	3.4...	3...	4.6...	6...	8.9...	1...	1.3...	1...	2.3...	2...
8	2	1	1	1E...	1...	1.2...	1...	2E...	2...	2.7...	3...	4.6...	5...
8	3	1	1	4.7...	5E...	5.5...	6...	7.7...	8...	9.5...	1...	1.5...	1...
8	4	1	1	5.5...	5...	5.9...	6E...	6.3...	6...	7E...	9...	1.1...	1...

Use case (2) : Plot CO-HE Rate Coeff. with TopCat

The TOPCAT interface shows the following details:

- Table List:**
 - 1: Col_CO-HE Rates -> All Temperatures
 - 2: Col_CO-HE Rates -> Single temperature
- Current Table Properties:**
 - Label: Col_CO-HE Rates -> All Temperatures
 - Location: Spectcol:Col_CO-HE Rates -> All Temperatures
 - Name: Col_CO-HE Rates -> All Temperatures



Let's work together

We are interested to work with the other VO-Tools

- Contact : yaye-awa.ba@obspm.fr
- Forum link : <http://forum.vamdc.org/>
- VAMDC Consortium website : <http://www.vamdc.org/>