

SPECTCOL : New interface improved with the query store connection

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SPECTCOL

- A graphical tool implemented in JavaFx.
- 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).
- Interoperability with other VO-tools (Topcat)
- Connection with the query store

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

SPECTCOL main panel

Import Panel

Search Panel

The screenshot displays the Spectcol FX software interface. At the top, there is an 'Import data from file' section with a 'Browse...' button and a 'File path:' input field. Below this is the 'Search VAMDC database' section, which includes a 'Databases to search:' dropdown menu set to 'VAMDC Nodes'. The search criteria are defined in the 'Form' section, with 'Collision & Transition' selected. The 'Form' fields include 'Nuclear spin' (set to '_any_'), 'Molecular species InChiKey', 'Molecular stoichiometric formula' (set to 'CO'), 'Ion charge', 'Atomic symbol', and 'Particle name'. A 'Selected databases' list on the right shows 'BASECOL2015: VAMDC-TAP ir' and 'CDMS'. Below the search form is the 'Transitions' table, which lists search results with columns for Comment, Source, Structural formula, Stoichiometric formula, Spin, and InChI key. Below the transitions table is the 'Collisions' table, which lists search results with columns for Comment, Source, Target struct..., Target stoic..., Target spin, Target InChi..., Collider stru..., Collider stoic..., Collider spin, and Collider InCh....

	Comment	Source	Structural formula	Stoichiometric formula	Spin	InChI key
1	29501- v2*:C-13-O; \$v=0\$	CDMS 2018-06-26 00:0...	C-13-O	CO		UGFAIRIUMAVXCW-OUBT...
2	30503- v 1:C-13-O-17; ...	CDMS 2018-06-26 00:0...	C-13-O-17	CO		UGFAIRIUMAVXCW-ZDOI...
3	29503- v 1:CO-17; \$v=0\$	CDMS 2018-06-26 00:0...	CO-17	CO		UGFAIRIUMAVXCW-VQEH...
4	28503- v 1:CO; \$v=0\$	CDMS 2018-06-26 00:0...	CO	CO		UGFAIRIUMAVXCW-UHFF...
5	28512- v1*:CO; \$v=1,2...	CDMS 2018-06-26 00:0...	CO	CO		UGFAIRIUMAVXCW-UHFF...
6	30502- v 1:CO-18; \$v=0\$	CDMS 2018-06-26 00:0...	CO-18	CO		UGFAIRIUMAVXCW-HQM...
7	31502- v 1:C-13-O-18; ...	CDMS 2018-06-26 00:0...	C-13-O-18	CO		UGFAIRIUMAVXCW-RGIGP...

	Comment	Source	Target struct...	Target stoic...	Target spin	Target InChi ...	Collider stru...	Collider stoic...	Collider spin	Collider InCh.
1	Rotational de...	BASECOL2015...	CO	CO		UGFAIRIUMAV...	H	H		YZCKVEUIGO...
2	Vibrational de...	BASECOL2015...	CO	CO		UGFAIRIUMAV...	H	H		YZCKVEUIGO...
3	Rotational de...	BASECOL2015...	CO	CO		UGFAIRIUMAV...	HE	HE		SWQJXJQGLNC...
4	Rotational de...	BASECOL2015...	CO	CO		UGFAIRIUMAV...	H\$ 2\$	H2	ORTHO	UFHFLCQGNY...
5	Vibrational de...	BASECOL2015...	CO	CO		UGFAIRIUMAV...	HE	HE		SWQJXJQGLNC...
6	Rotational de...	BASECOL2015...	CO	CO		UGFAIRIUMAV...	H\$ 2\$	H2	PARA	UFHFLCQGNY...
7	Rotational exc...	BASECOL2015...	CO	CO		UGFAIRIUMAV...	H\$ 2\$	H2	ORTHO	UFHFLCQGNY...

Spectroscopic data results

Collisional data results

Selected database

Buttons to Manipulate data

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)

Import data from file
Browse... File path: path Collision Transition Collision & Transition Import

Search VAMDC database
Databases to search: VAMDC Nodes

Species Collision & Transition

Form

Nuclear spin

Molecular species InChIKey

Molecular stoichiometric formula

Ion charge

Atomic symbol

Particle name

Submit query Cancel

Selected databases

Transitions

Comment	Source	Structural formula	Stoichiometric formula	Spin	InChI key
Transition table is empty					

Collisions

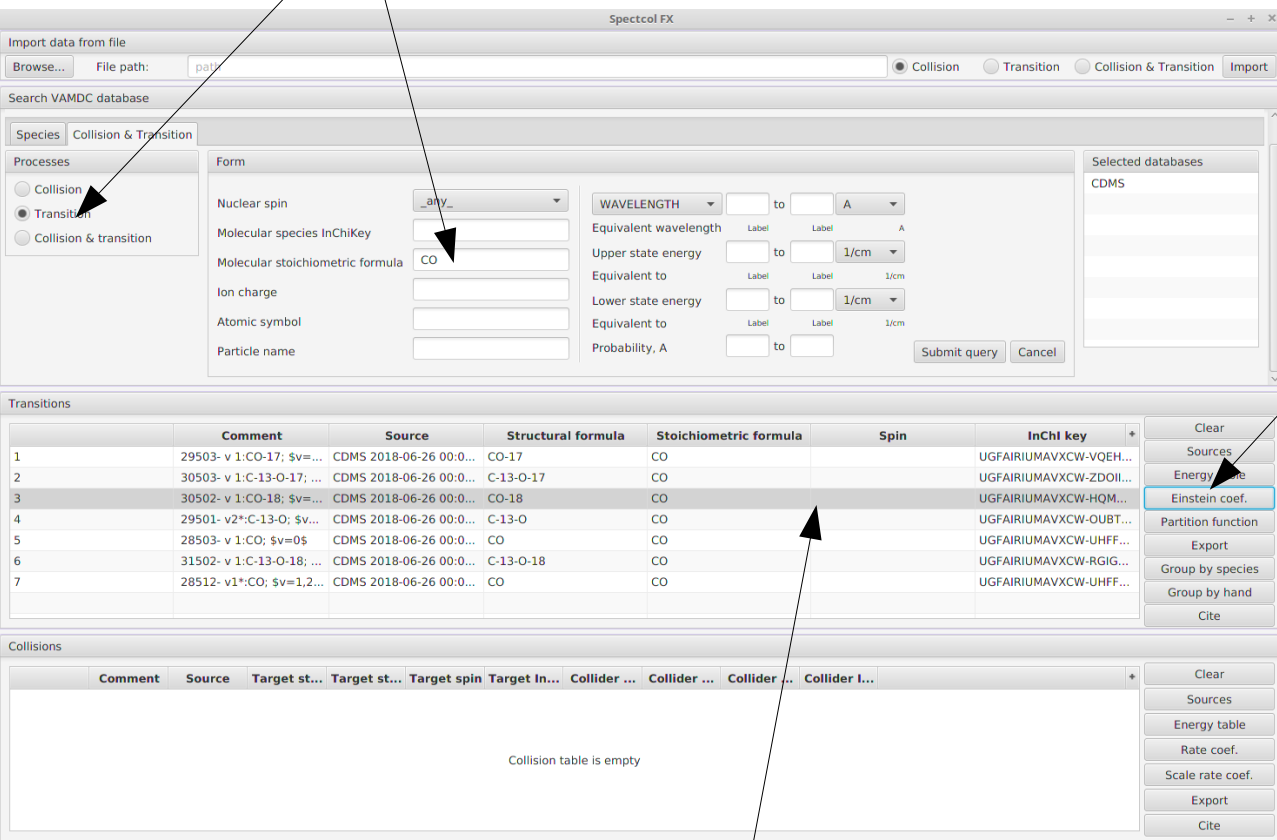
Comment	Source	Target struct...	Target stoic...	Target spin	Target InChI ...	Collider stru...	Collider stoic...	Collider spin	Collider InCh...
Collision table is empty									

	Title	Description	Status	Ivold
<input type="checkbox"/>	UMIST Database...	Reaction rate co...	active	ivo://vamdc/UDFA
<input type="checkbox"/>	Carbon Dioxide ...	Carbon Dioxide ...	active	ivo://vamdc/cds...
<input type="checkbox"/>	BASECOL2015: ...	This database, c...	active	ivo://vamdc/bas...
<input type="checkbox"/>	Stark-b	Database for "St...	active	ivo://vamdc/star...
<input type="checkbox"/>	VALD sub-set in ...	The part of Vien...	active	ivo://vamdc/val...
<input type="checkbox"/>	Chianti	Chianti consists ...	active	ivo://vamdc/chia...
<input type="checkbox"/>	TIPbase : VAMD...	TIPbase lists fin...	active	ivo://vamdc/TIP...
<input type="checkbox"/>	LXcat	An open-access ...	active	ivo://vamdc/lxcat
<input type="checkbox"/>	VAMDC species-...	This Database c...	active	ivo://vamdc/Va...
<input type="checkbox"/>	TOPbase : VAM...	TOPbase lists LS...	active	ivo://vamdc/TOP...
<input type="checkbox"/>	AMDIS Ionization	Ionization cross ...	active	ivo://vamdc/am...
<input type="checkbox"/>	GeCaSDa: Gema...	Calculated line l...	active	ivo://vamdc/dijo...
<input type="checkbox"/>	BASECOL: VAMD...	This database, c...	active	ivo://vamdc/bas...
<input type="checkbox"/>	Water internet A...	Database contai...	active	ivo://vamdc/wad...
<input type="checkbox"/>	TFMeCaSDa - CF...	Calculated line l...	active	ivo://vamdc/dijo...
<input type="checkbox"/>	OACT - LASP Dat...	Laboratorio di ...	active	ivo://vamdc/OA...
<input type="checkbox"/>	Belgrade electro...	Electron interac...	active	ivo://vamdc/em...
<input type="checkbox"/>	MeCaSDa - Meth...	Calculated line l...	active	ivo://vamdc/dijo...
<input type="checkbox"/>	Theoretical spec...	The Cagliari/Tou...	active	ivo://vamdc/OA-...
<input type="checkbox"/>	VALD (atoms)	The Vienna Ato...	active	ivo://vamdc/val...
<input type="checkbox"/>	NIST Atomic Spe...	This database p...	active	ivo://vamdc/nist...

Ok Quit

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

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

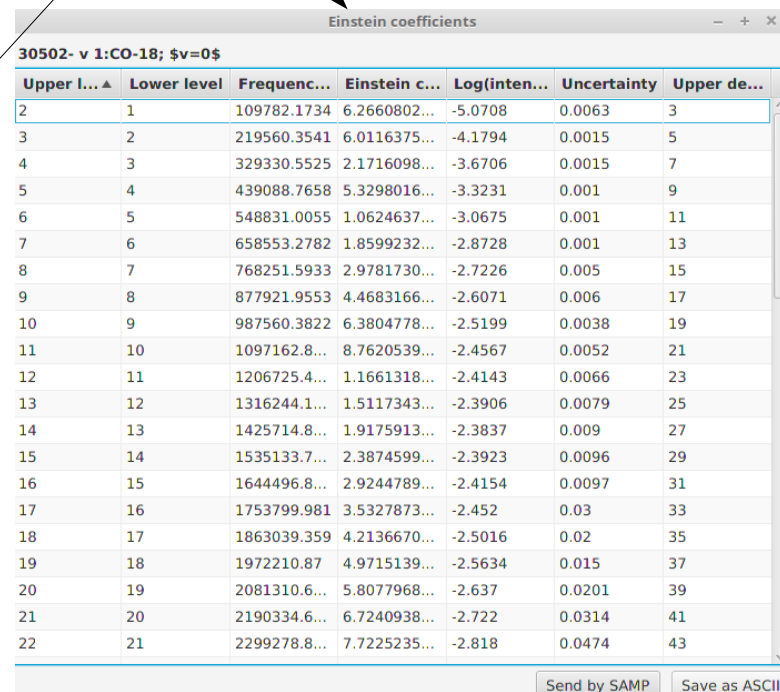


The screenshot shows the Spectcol FX search interface. The 'Collision & Transition' tab is active. The 'Processes' section has 'Transition' selected. The 'Form' section has 'Molecular stoichiometric formula' set to 'CO'. The 'Transitions' table is visible below, showing search results for CO transitions.

	Comment	Source	Structural formula	Stoichiometric formula	Spin	InChI key
1	29503- v 1:CO-17; \$v=...	CDMS 2018-06-26 00:0...	CO-17	CO		UGFAIRIUAVXCW-VQEH...
2	30503- v 1:C-13-O-17; ...	CDMS 2018-06-26 00:0...	C-13-O-17	CO		UGFAIRIUAVXCW-ZDOI...
3	30502- v 1:CO-18; \$v=...	CDMS 2018-06-26 00:0...	CO-18	CO		UGFAIRIUAVXCW-HQM...
4	29501- v2*:C-13-O; \$v...	CDMS 2018-06-26 00:0...	C-13-O	CO		UGFAIRIUAVXCW-OUBT...
5	28503- v 1:CO; \$v=0\$	CDMS 2018-06-26 00:0...	CO	CO		UGFAIRIUAVXCW-UHFF...
6	31502- v 1:C-13-O-18; ...	CDMS 2018-06-26 00:0...	C-13-O-18	CO		UGFAIRIUAVXCW-RGIG...
7	28512- v1*:CO; \$v=1,2...	CDMS 2018-06-26 00:0...	CO	CO		UGFAIRIUAVXCW-UHFF...

3. Select a spectroscopic dataset

4. Display Einstein table



The screenshot shows the 'Einstein coefficients' window for the transition '30502- v 1:CO-18; \$v=0\$'. The table displays Einstein coefficients for various upper and lower levels.

Upper l...	Lower level	Frequenc...	Einstein c...	Log(inten...	Uncertainty	Upper de...
2	1	109782.1734	6.2660802...	-5.0708	0.0063	3
3	2	219560.3541	6.0116375...	-4.1794	0.0015	5
4	3	329330.5525	2.1716098...	-3.6706	0.0015	7
5	4	439088.7658	5.3298016...	-3.3231	0.001	9
6	5	548831.0055	1.0624637...	-3.0675	0.001	11
7	6	658553.2782	1.8599232...	-2.8728	0.001	13
8	7	768251.5933	2.9781730...	-2.7226	0.005	15
9	8	877921.9553	4.4683166...	-2.6071	0.006	17
10	9	987560.3822	6.3804778...	-2.5199	0.0038	19
11	10	1097162.8...	8.7620539...	-2.4567	0.0052	21
12	11	1206725.4...	1.1661318...	-2.4143	0.0066	23
13	12	1316244.1...	1.5117343...	-2.3906	0.0079	25
14	13	1425714.8...	1.9175913...	-2.3837	0.009	27
15	14	1535133.7...	2.3874599...	-2.3923	0.0096	29
16	15	1644496.8...	2.9244789...	-2.4154	0.0097	31
17	16	1753799.981	3.5327873...	-2.452	0.03	33
18	17	1863039.359	4.2136670...	-2.5016	0.02	35
19	18	1972210.87	4.9715139...	-2.5634	0.015	37
20	19	2081310.6...	5.8077968...	-2.637	0.0201	39
21	20	2190334.6...	6.7240938...	-2.722	0.0314	41
22	21	2299278.8...	7.7225235...	-2.818	0.0474	43

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

Einstein coefficients

30502- v 1:CO-18; \$v=0\$

Upper l...	Lower level	Frequenc...	Einstein c...	Log(inten...	Uncertainty	Upper de...
2	1	109782.1734	6.2660802...	-5.0708	0.0063	3
3	2	219560.3541	6.0116375...	-4.1794	0.0015	5
4	3	329330.5525	2.1716098...	-3.6706	0.0015	7
5	4	439088.7658	5.3298016...	-3.3231	0.001	9
6	5	548831.0055	1.0624637...	-3.0675	0.001	11
7	6	658553.2782	1.8599232...	-2.8728	0.001	13
8	7	768251.5933	2.9781730...	-2.7226	0.005	15
9	8	877921.9553	4.4683166...	-2.6071	0.006	17
10	9	987560.3822	6.3804778...	-2.5199	0.0038	19
11	10	1097162.8...	8.7620539...	-2.4567	0.0052	21
12	11	1206725.4...	1.1661318...	-2.4143	0.0066	23
13	12	1316244.1...	1.5117343...	-2.3906	0.0079	25
14	13	1425714.8...	1.9175913...	-2.3837	0.009	27
15	14	1535133.7...	2.3874599...	-2.3923	0.0096	29
16	15	1644496.8...	2.9244789...	-2.4154	0.0097	31
17	16	1753799.981	3.5327873...	-2.452	0.03	33
18	17	1863039.359	4.2136670...	-2.5016	0.02	35
19	18	1972210.87	4.9715139...	-2.5634	0.015	37
20	19	2081310.6...	5.8077968...	-2.637	0.0201	39
21	20	2190334.6...	6.7240938...	-2.722	0.0314	41
22	21	2299278.8...	7.7225235...	-2.818	0.0474	43

Send by SAMP Save as ASCII

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: SpectcolFx:Sp_CO_Einstein
Name: Sp_CO_Einstein
Rows: 60
Columns: 8
Sort Order:
Row Subset: All
Activation Actions: 0 / 0

SAMP

Messages: Clients:

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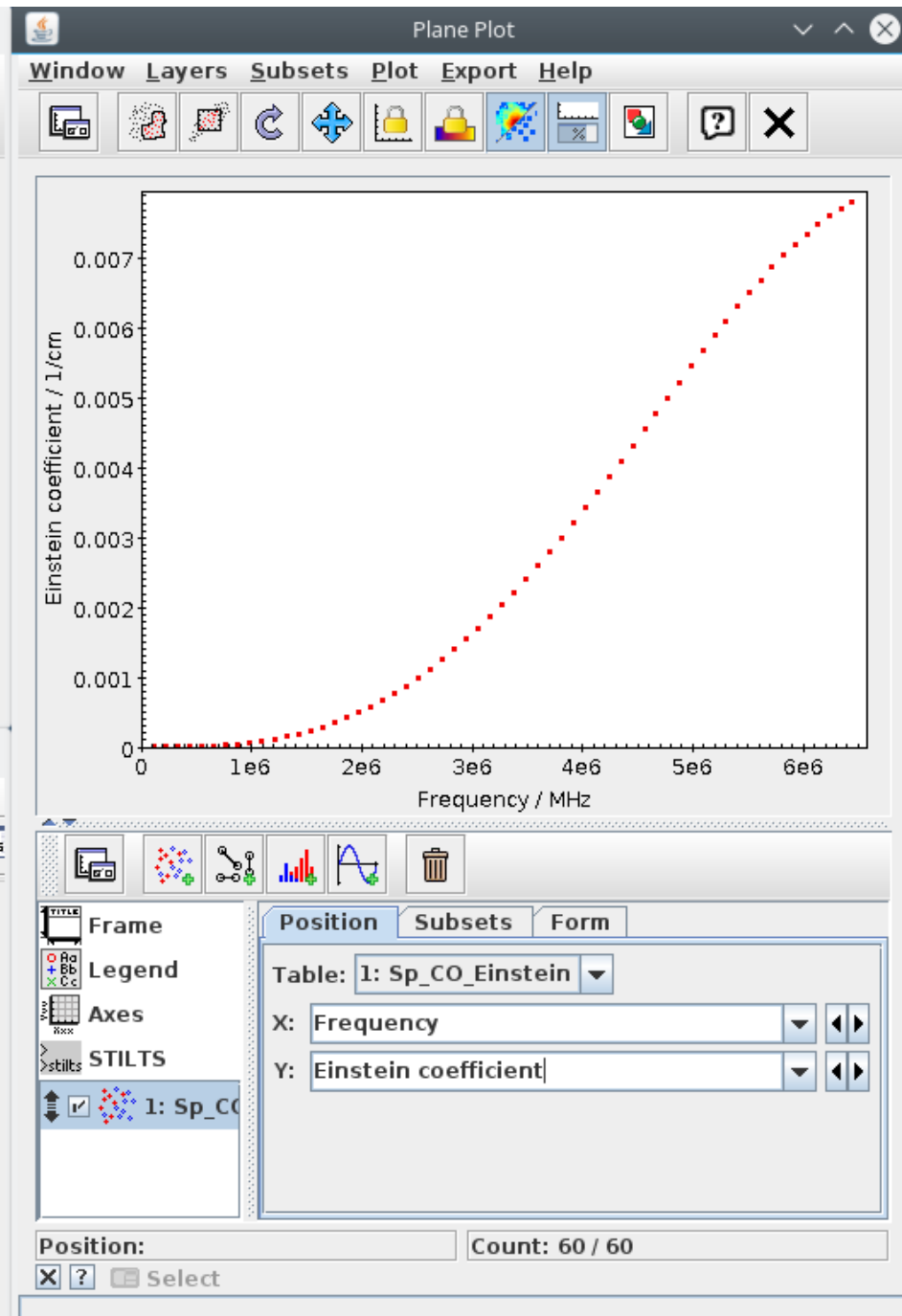
Use case (1) : Plot CO Einstein Coeff. with TopCat

TOPCAT(1): Table Browser

Window Subsets Help

Table Browser for 1: Sp_CO_Einstein

	Index	Upper ...	Lower l...	Frequency	Einstein coeff...	log(intensi...	Uncertainty
1	1	2	1	1,097822E5	6,266080E-8	-5,0708	0,0063
2	2	3	2	2,195604E5	6,011638E-7	-4,1794	0,0015
3	3	4	3	3,293306E5	2,171610E-6	-3,6706	0,0015
4	4	5	4	4,390888E5	5,329802E-6	-3,3231	0,001
5	5	6	5	5,488310E5	1,062464E-5	-3,0675	0,001
6	6	7	6	6,585533E5	1,859923E-5	-2,8728	0,001
7	7	8	7	7,682516E5	2,978173E-5	-2,7226	0,005
8	8	9	8	8,779220E5	4,468317E-5	-2,6071	0,006
9	9	10	9	9,875604E5	6,380478E-5	-2,5199	0,0038
10	10	11	10	1,097163E6	8,762054E-5	-2,4567	0,0052
11	11	12	11	1,206725E6	0,00012	-2,4143	0,0066
12	12	13	12	1,316244E6	0,00015	-2,3906	0,0079
13	13	14	13	1,425715E6	0,00019	-2,3837	0,009
14	14	15	14	1,535134E6	0,00024	-2,3923	0,0096
15	15	16	15	1,644497E6	0,00029	-2,4154	0,0097
16	16	17	16	1,753960E6	0,00035	-2,452	0,01



TOPCAT

File Views Graphics Joins Windows VO Interop Help

Table List

- 1: Sp_CO_Einstein

Current Table Properties

Label: Sp_CO_Einstein

Location: SpectcolFx:Sp_CO_Einstein

Name: Sp_CO_Einstein

Rows: 60

Columns: 8

Sort Order:

Row Subset: All

Activation Actions: 0 / 0

SAMP

Messages:

Clients:

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SPECTCOL : Automatic data citation

Spectcol can communicate with the query store and show data citation.

- Retrieve the query token generated by the node.
- Make an association with the query store and get the UUID
- Get the citation linked to the UUID

Use case (2) : Data citation

Same procedure than the spectroscopy to search collisional data :

1. Select the new BASECOL database
2. Search the collision CO-HE
3. Select a dataset
4. Display the link of the citation

The screenshot shows the Spectrol FX software interface. The 'Search VAMDC database' section is active, with 'Collision & transition' selected. The search criteria are: Molecular species InChiKey (empty), Molecular stoichiometric formula (CO), Ion charge (empty), Atomic symbol (He), and Particle name (empty). The 'Collisions' table is displayed below, showing two results:

	Comment	Source	Target st...	Target st...	Target spin	Target In...	Collider s...	Collider s...	Collider s...	Collider I. +
1	Rotational ...	BASECOL2...	CO	CO		UGFAIRIU...	HE	HE		SWQJXJOG...
2	Vibrational...	BASECOL2...	CO	CO		UGFAIRIU...	HE	HE		SWQJXJOG...

The 'QueryStore cite url' dialog box is shown, displaying the citation URL: <http://vm-calc-lerma01.obspm.fr:8080/QueryStore/browse/references/uuid=fd8d0729-7857-417b-8ae8-5f6ff510b23a>. An arrow points from the 'Cite' button in the Spectrol FX interface to this dialog box.

Use case (2) : Data citation

Copy the link in a browser
Get data citation

[Get a DOI](#)

Data source : http://basecoltap2015.vamdc.org/12_07/

Data source version : 2018-05-03

Query : `select * where (target.moleculestoichiometricformula = 'co')`

Query identifier : 701a8de8-f073-42b0-a1af-463bd80e447b

Query result : [XSAMS file](#)

XSAMS version : 12.07

Query result downloaded on (UTC+1) :

- 2018-6-26 0:30:05



References

- [Reference name in bibtex](#) : BBAS0
- [Error](#): title is missing, please check bibtex source code to get more information.

- [Title](#) : The rotational excitation of CO by H₂
- [Journal](#) : JPhB
- [Authors](#) : Flower,D.~R.
- [Pages](#) : 2731,2738
- [Volume](#) : 34
- [Year](#) : 2001
- [Reference name in bibtex](#) : BBAS62

- [Title](#) : Quantum Mechanical Study of Rotational and Vibrational Transitions in CO Induced by H Atoms

[Switch to Bibtex](#)



SPECTCOL : Matching data

Spectcol can combine the spectroscopic and collisional data.

- Query both databases : spectroscopic and collisional databases. Ex: Basecol and JPL
- Select a dataset of each of them
- Select the quantum numbers and let spectcol do the job

Use case (3) : Matching data

1. query databases and select « group by species »
Or « group by hand » buttons

	Comment	Source	Structural formula	Stoichiometric formula	Spin	InChI key
1	29501- v1-C-13-O-9...	CDMS 2018-06-26 00.0...	C-13-O	CO		UGFAIRIUMAVXCW-UHFFFA...
2	30503- v1-C-13-O-17...	CDMS 2018-06-26 00.0...	C-13-O-17	CO		UGFAIRIUMAVXCW-ZDOL...
3	29503- v1-CO-17; \$v=0\$	CDMS 2018-06-26 00.0...	CO-17	CO		UGFAIRIUMAVXCW-VOEH...
4	28503- v1-CO; \$v=0\$	CDMS 2018-06-26 00.0...	CO	CO		UGFAIRIUMAVXCW-UHFF...
5	28512- v1*CO; \$v=1,2,3\$	CDMS 2018-06-26 00.0...	CO	CO		UGFAIRIUMAVXCW-UHFF...
6	30502- v1-CO-18; \$v=0\$	CDMS 2018-06-26 00.0...	CO-18	CO		UGFAIRIUMAVXCW-HOM...
7	31502- v1-C-13-O-18...	CDMS 2018-06-26 00.0...	C-13-O-18	CO		UGFAIRIUMAVXCW-RGGP...

2. Select the datasets

	Comment	Source	Target str...	Target sto...	Target spin	Target InC...	Collider str...	Collider sto...	Collider spin	Collider In...
1	Rotational de-excitation ...	BASECOL20...	CO	CO		UGFAIRIUM... H	H			YZCKVEUG...
2	Vibrational de-excitation ...	BASECOL20...	CO	CO		UGFAIRIUM... H	H			YZCKVEUG...
3	Rotational de-excitation ...	BASECOL20...	CO	CO		UGFAIRIUM... HE	HE			SWQJXJOG...
4	Rotational de-excitation ...	BASECOL20...	CO	CO		UGFAIRIUM... H _{S_2}	H2	ORTHO		UFHFLCOG...
5	Vibrational de-excitation ...	BASECOL20...	CO	CO		UGFAIRIUM... HE	HE			SWQJXJOG...
6	Rotational de-excitation ...	BASECOL20...	CO	CO		UGFAIRIUM... H _{S_2}	H2	PARA		UFHFLCOG...
7	Rotational excitation of C...	BASECOL20...	CO	CO		UGFAIRIUM... H _{S_2}	H2	ORTHO		UFHFLCOG...

3. Choose the quantum numbers

	Comment	Source	Target str...	Target sto...	Target spin	Target InC...	Collider str...	Collider sto...	Collider spin	Collider In...
1	Rotational de-excitation ...	BASECOL20...	CO	CO		UGFAIRIUM... H	H			YZCKVEUG...
2	Vibrational de-excitation ...	BASECOL20...	CO	CO		UGFAIRIUM... H	H			YZCKVEUG...
3	Rotational de-excitation ...	BASECOL20...	CO	CO		UGFAIRIUM... HE	HE			SWQJXJOG...
4	Rotational de-excitation ...	BASECOL20...	CO	CO		UGFAIRIUM... H _{S_2}	H2	ORTHO		UFHFLCOG...
5	Vibrational de-excitation ...	BASECOL20...	CO	CO		UGFAIRIUM... HE	HE			SWQJXJOG...
6	Rotational de-excitation ...	BASECOL20...	CO	CO		UGFAIRIUM... H _{S_2}	H2	PARA		UFHFLCOG...
7	Rotational excitation of C...	BASECOL20...	CO	CO		UGFAIRIUM... H _{S_2}	H2	ORTHO		UFHFLCOG...

Index	Energy [1...	Degeneracy	ElecStateLabel	v	J	I	F1	F	parity	kronigPar
1	0.0	1.0	X	0	0					
2	3.845033	3.0	X	0	1					
3	11.534953	5.0	X	0	2					
4	23.069466	7.0	X	0	3					
5	38.448131	9.0	X	0	4					
6	57.67036	11.0	X	0	5					
7	80.735419	13.0	X	0	6					
8	107.642427	15.0	X	0	7					
9	138.390355	17.0	X	0	8					
10	172.978079	19.0	X	0	9					

Use case (3) : Ouput

Matching result

▼ State energy and quantum numbers

Index	Energy [1/cm]	Degeneracy	ElecStateLabel	v	J	I	F1	F	parity	kronigParity	asSym
1	0.0	1.0			0						
2	3.845033	3.0			1						
3	11.534953	5.0			2						

▼ Rate coefficients

I1	F1	I2	F2	5.0	10.0	20.0	30.0	40.0	50.0	60.0	70.0	80.0	90.0	100.0
2	1	1	1	1.78E-10	1.93E-10	2.02E-10	2.09E-10	2.15E-10	2.2E-10	2.25E-10	2.28E-10	2.32E-10	2.34E-10	2.37E-10
3	1	1	1	9.74E-11	9.31E-11	8.25E-11	7.69E-11	7.41E-11	7.26E-11	7.18E-11	7.15E-11	7.13E-11	7.11E-11	7.1E-11

▼ Einstein coefficients

Upper le...	Lower le...	Frequency [MHz]	Einstein coeff	Log (intensity)	Uncertainty	Upper degeneracy
2	1	115271.2018	7.20360334988E-8	-5.0105	5.0E-4	3
3	2	230538.0	6.91061226474E-7	-4.1197	5.0E-4	5
4	3	345795.9899	2.49663664213E-6	-3.6118	5.0E-4	7

▼ Collider state energy and quantum numbers

Index	Energy [1/cm]	Degeneracy	parity	J	F	M	Kappa	term type	I	S	j	S2	K
1	0.0			0.0				LS	0	0.0			

▼ Partition function withCDMS degeneracy

T [K]	Q
1.072	1.01721581835
1.148	1.02422837677
1.22	1.03241102522

Export

* Energy Rate coefficients Einstein coefficients Collider energy Partition function Save as Ascii

* Save as Radex Save as Xsams Save file

Spectroscopic data

Collisional data

Radex File

XSAMS File

Ascii File

Contact

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- VAMDC Consortium website : <http://www.vamdc.org/>

Thank you