

Spectcol

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Speaker : Nicolas Moreau

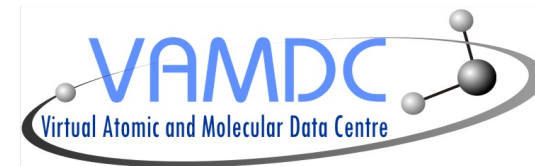
Lerma, Paris Observatory

Spectcol overview



- Java application
- Dedicated to spectroscopic and collisional data manipulation and combination
- Uses the VAMDC infrastructure to query several databases :
 - Basecol for collisional data
 - JPL, CDMS and Hitran for spectroscopic data
- Uses XSAMS format to read data
- Provides export functionalities to other formats

Main window



SPECTCOL

Help

Import data from file

Browse... File path: collisions transitions

Search VAMDC databases

Databases to search: BASECOL CDMS HITRAN JPL

Species search **Transitions search** Collision search

Nuclear spin: Wavelength to

Molecular species InChiKey: Equivalent Wavelength to

Molecular stoichiometric formula: Upper state energy: to

Ion charge: Equivalent to to

Atomic symbol: Lower state energy: to

Particle name: Probability, A: to

Transitions

	comment	source	structural formula	stoichiometric fo...	spin	InChi key
1	27505- v1*:C-13-N; \$v=0\$	CDMS 2014-06-1...	C-13-N	CN		JEVCWSUVFOYBF...
2	27506- v1*:CN-15; \$v=0\$	CDMS 2014-06-1...	CN-15	CN		JEVCWSUVFOYBF...
3	26504- v1*:CN; \$v = 0, 1\$	CDMS 2014-06-1...	CN	CN		JEVCWSUVFOYBF...
4	28505- v1*:C-13-N-15; \$v=0\$	CDMS 2014-06-1...	C-13-N-15	CN		JEVCWSUVFOYBF...

Clear Sources Energy table Einstein coef. Partition func. Export Group by hand Group by species

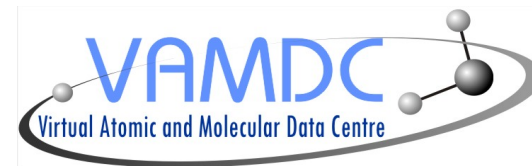
Collisions

	comment	source	target stru...	target stoi...	target spin	target InCh...	collider str...	collider stoi...	collider spin	collider InC...
1	Rotational de-excitation of fine levels of CN by He (Lique et...	BASECOL 2...	CN	CN		JEVCWSUV...	HE	HE		SWQJXJOG...
2	Hyperfine collisional excitation of CN by He - 5K to 30K (Liq...	BASECOL 2...	CN	CN		JEVCWSUV...	HE	HE		SWQJXJOG...

Clear Sources Energy table Rate coef. Scale Rate coef. Export



Data visualization (1/2)



Energy table

Energy table - CHO+ - FIRPXVMTWVPCB-UHFFFAOYSA-N - CDM...

29505- v 1:HOC+; \$v2=1\$

st...	en...	de...	El...	J	v1	v2	v3	F	F1	F2	pa...	kr...	r	l2	As...
1	2...	3X		1	0	1	0					e		1	
2	2...	3X		1	0	1	0					f		1	
3	2...	5X		2	0	1	0					e		1	
4	2...	5X		2	0	1	0					f		1	
5	2...	7X		3	0	1	0					e		1	
6	2...	7X		3	0	1	0					f		1	
7	2...	9X		4	0	1	0					e		1	
8	2...	9X		4	0	1	0					f		1	
9	2...	11X		5	0	1	0					e		1	
10	2...	11X		5	0	1	0					f		1	
11	3...	13X		6	0	1	0					e		1	
12	3...	13X		6	0	1	0					f		1	
13	3...	15X		7	0	1	0					e		1	
14	3...	15X		7	0	1	0					f		1	
15	3...	17X		8	0	1	0					e		1	
16	3...	17X		8	0	1	0					f		1	
17	3...	19X		9	0	1	0					e		1	
18	3...	19X		9	0	1	0					f		1	
19	4...	21X		10	0	1	0					e		1	
20	4...	21X		10	0	1	0					f		1	
21	4...	23X		11	0	1	0					e		1	
22	4...	23X		11	0	1	0					f		1	
23	4...	25X		12	0	1	0					e		1	
24	4...	25X		12	0	1	0					f		1	
25	5...	27X		13	0	1	0					e		1	

plot energy graph save as ASCII

Einstein coefficients

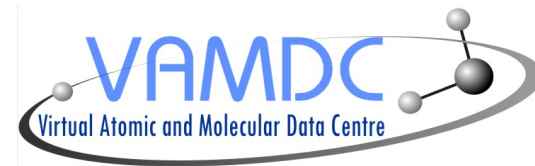
Einstein coefficients

29505- v 1:HOC+; \$v2=1\$

uppe...	lower le...	frequen...	Einstein...	log(inte...	uncertai...	upper d...
3	2	1037.5...	4.9908...	-6.9497	0.0073	3
4	2	178719...	1.5305...	-2.4835	0.0223	5
5	4	3112.0...	4.4891...	-6.2634	0.0211	5
5	3	180793...	1.5845...	-2.4736	0.0223	5
6	4	268072...	6.5585...	-1.897	0.0279	7
7	6	6222.6...	1.7942...	-5.8352	0.0403	7
7	5	271182...	6.7896...	-1.8873	0.0279	7
8	6	357417...	0.0017...	-1.5208	0.0279	9
9	8	10367...	4.9800...	-5.5294	0.0629	9
9	7	361562...	0.0017...	-1.5113	0.0279	9
10	8	446752...	0.0034...	-1.2477	0.023	11
11	10	15545...	1.1192...	-5.2977	0.0864	11
11	9	451930...	0.0035...	-1.2386	0.023	11
12	10	536075.1	0.0061...	-1.0388	0.02	13
13	12	21753...	2.1905...	-5.1169	0.1078	13
13	11	542282...	0.0063...	-1.0301	0.02	13
14	12	625381...	0.0099...	-0.875	0.02	15
15	14	28988...	3.8877...	-4.974	0.1239	15
15	13	632616...	0.0103...	-0.8668	0.02	15
16	14	714670...	0.0151...	-0.7455	0.0162	17
17	16	37246...	6.4142...	-4.861	0.1319	17
17	15	722929...	0.0156...	-0.7378	0.0162	17
18	16	803939...	0.0217...	-0.6434	0.02	19
19	18	46525...	1.0000...	-4.7726	0.1309	19
19	17	813217...	0.0224...	-0.6363	0.02	19

save as ASCII

Data visualization (2/2)



Partition function

Partition function table

Partition function with CDMS degeneracy

T [K]	Q
1.072	1.05463336423
1.148	1.07125426103
1.23	1.0914931701
1.318	1.11562017273
1.413	1.1441335958
1.514	1.17686824773
1.622	1.21419713002
1.738	1.25650108349
1.862	1.30377265206
1.995	1.35635000285
2.138	1.41457910925
2.291	1.47839177928
2.455	1.54812706711
2.63	1.62370667308
2.725	1.66513860396
2.818	1.70592815943
3.02	1.79518168207
3.236	1.89142263001
3.467	1.99505574941
3.715	2.10694956592
3.981	2.22753503492
4.266	2.3572480179
4.571	2.49652821571
4.898	2.64627688478
5.0	2.69306227319

save as ASCII

Rate coefficients

Rate coefficients - Rotational collisional de-excitation rate coefficients of N₂H⁺ by He, 5K < T < 50K (Daniel ...)

Rotational collisional de-excitation rate coefficients of N₂H⁺ by He, 5K < T < 50K (Daniel & al. 2005)

l1	F1	l2	F2	5.0	10.0	20.0	30.0	40.0	50.0
2	1	1	1	1.32E-10	1.15E-10	1.03E-10	9.76E-11	9.44E-11	9.23E-11
3	1	1	1	7.05E-11	6.26E-11	5.09E-11	4.36E-11	3.88E-11	3.55E-11
3	2	1	1	1.82E-10	1.74E-10	1.59E-10	1.5E-10	1.44E-10	1.4E-10
4	1	1	1	3.88E-11	3.63E-11	3.09E-11	2.74E-11	2.49E-11	2.32E-11
4	2	1	1	1.01E-10	1.01E-10	9.03E-11	8.13E-11	7.48E-11	7.01E-11
4	3	1	1	1.94E-10	1.81E-10	1.63E-10	1.55E-10	1.51E-10	1.49E-10
5	1	1	1	2.65E-11	2.31E-11	1.98E-11	1.8E-11	1.68E-11	1.6E-11
5	2	1	1	6.98E-11	6.84E-11	6.35E-11	5.96E-11	5.69E-11	5.49E-11
5	3	1	1	1.42E-10	1.4E-10	1.3E-10	1.21E-10	1.14E-10	1.09E-10
5	4	1	1	2.02E-10	1.97E-10	1.87E-10	1.79E-10	1.74E-10	1.71E-10
6	1	1	1	2.13E-11	2.18E-11	2.12E-11	2.04E-11	1.97E-11	1.92E-11
6	2	1	1	7.15E-11	6.94E-11	6.42E-11	5.96E-11	5.6E-11	5.3E-11
6	3	1	1	1.15E-10	1.13E-10	1.04E-10	9.62E-11	8.97E-11	8.47E-11
6	4	1	1	1.2E-10	1.22E-10	1.18E-10	1.13E-10	1.09E-10	1.05E-10
6	5	1	1	1.41E-10	1.4E-10	1.41E-10	1.42E-10	1.43E-10	1.45E-10
7	1	1	1	2.29E-11	2.23E-11	2.04E-11	1.87E-11	1.73E-11	1.61E-11
7	2	1	1	5.76E-11	5.84E-11	5.48E-11	5.09E-11	4.77E-11	4.51E-11
7	3	1	1	6.96E-11	7.3E-11	7.15E-11	6.81E-11	6.5E-11	6.23E-11
7	4	1	1	9.01E-11	9.16E-11	9.04E-11	8.77E-11	8.48E-11	8.22E-11
7	5	1	1	1.04E-10	1.06E-10	1.07E-10	1.05E-10	1.03E-10	1.01E-10
7	6	1	1	1.24E-10	1.23E-10	1.23E-10	1.24E-10	1.27E-10	1.29E-10

save as ASCII

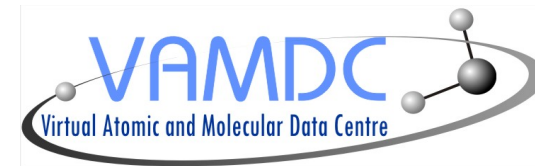
Combining spectroscopic and collisional data

- We have the possibility to do a matching of levels between isoelectronic molecules
- In the example below we have spectroscopic data for HCO^+ , collisional data for $\text{N}_2\text{H}^+ - \text{He}$
- HCO^+ and N_2H^+ are isoelectronic $\rightarrow \text{N}_2\text{H}^+ - \text{He} \sim \text{HCO}^+ - \text{He}$

Transitions						
	comment	source	structural formula	stoichiometric f...	spin	InChI key
1	29515- v1*:HCO+; \$nu_2\$ IR band	CDMS 2014-07-...	HCO+	CHO+		XPRMKTHGXOVK...
2	29508- v2*:HCO+; \$v2=1\$	CDMS 2014-07-...	HCO+	CHO+		XPRMKTHGXOVK...
3	30505- v1:HCO-17+; \$v=0\$	CDMS 2014-07-...	HCO-17+	CHO+		XPRMKTHGXOVK...
4	31506- v1:HCO-18+; \$v=0\$	CDMS 2014-07-...	HCO-18+	CHO+		XPRMKTHGXOVK...
5	31508- v2*:DC-13-0+; \$v=0\$	CDMS 2014-07-...	DC-13-0+	CHO+		XPRMKTHGXOVK...
6	30504- v2*:HC-13-0+; \$v=0\$	CDMS 2014-07-...	HC-13-0+	CHO+		XPRMKTHGXOVK...
7	29507- v2*:HCO+; \$v=0\$	CDMS 2014-07-...	HCO+	CHO+		XPRMKTHGXOVK...
8	30510- v3*:DCO+; \$v=0\$	CDMS 2014-07-...	DCO+	CHO+		XPRMKTHGXOVK...
9	32505- v1*:DCO-18+; \$v=0\$	CDMS 2014-07-...	DCO-18+	CHO+		XPRMKTHGXOVK...
10	30506- v1*:DOC+; \$v=0\$	CDMS 2014-07-...	DOC+	CHO+		FIRPXVMTWVP...
11	29505- v1:HOC+; \$v2=1\$	CDMS 2014-07-...	HOC+	CHO+		FIRPXVMTWVP...

Collisions										
	comment	source	target stru...	target stoi...	target spin	target InCh...	collider str...	collider stoi...	collider spin	collider InC...
1	Rotational collisional de-excitation rate coefficients of N\$...	BASECOL 2...	\$N_2H^+ \$	HN2+		JJGRMHOSH...	HE	HE		SWQXJUGL...
2	Hyperfine collisional excitation rate coefficients of N\$ 2\$H...	BASECOL 2...	\$N_2H^+ \$	HN2+		JJGRMHOSH...	HE	HE		SWQXJUGL...
3	Rotational excitation of N\$ 2\$H\$^+ \$ by He (Green, 1975)	BASECOL 2...	\$N_2H^+ \$	HN2+		JJGRMHOSH...	HE	HE		SWQXJUGL...

Combining spectroscopic and collisional data



1. Dataset selection

Species <2>

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

Transitions

	comment	source	structural formula	stoichiometric f...	spin	InChI key
1	29515-v1*:HC...	CDMS 2014-07-...	HCO+	CHO+		XPRMKTHGXOVK...
2	29508-v2*:HC...	CDMS 2014-07-...	HCO+	CHO+		XPRMKTHGXOVK...
3	30505-v1*:HC...	CDMS 2014-07-...	HCO-17+	CHO+		XPRMKTHGXOVK...
4	31506-v1*:HC...	CDMS 2014-07-...	HCO-18+	CHO+		XPRMKTHGXOVK...
5	31508-v2*:DC...	CDMS 2014-07-...	DC-13-0+	CHO+		XPRMKTHGXOVK...
6	30504-v2*:HC...	CDMS 2014-07-...	HC-13-0+	CHO+		XPRMKTHGXOVK...
7	29507-v2*:HC...	CDMS 2014-07-...	HCO+	CHO+		XPRMKTHGXOVK...
8	30510-v3*:DC...	CDMS 2014-07-...	DCO+	CHO+		XPRMKTHGXOVK...
9	32505-v1*:DC...	CDMS 2014-07-...	DCO-18+	CHO+		XPRMKTHGXOVK...
10	30506-v1*:DO...	CDMS 2014-07-...	DOC+	CHO+		FIRPXVMTWVP...
11	29505-v1*:HO...	CDMS 2014-07-...	HOC+	CHO+		FIRPXVMTWVP...

Collisions

	comment	source	target str...	target st...	target spin	target In...	collider st...	collider s...	collider s...	collider In...
1	Rotation...	BASECOL...	\$N_2H^+\$	HN2+		GRMHO...	HE	HE		SWQJXJ0...
2	Hyperfin...	BASECOL...	\$N_2H^+\$	HN2+		GRMHO...	HE	HE		SWQJXJ0...
3	Rotation...	BASECOL...	\$N_2H^+\$	HN2+		GRMHO...	HE	HE		SWQJXJ0...

Scaled collisions

	comment	source	target str...	target st...	target spin	target In...	collider st...	collider s...	collider s...	collider In...
1:f=1.44	Scaled r...	BASECOL...	\$N_2H^+\$	HN2+		GRMHO...	HE	HE		SWQJXJ0...

Show selection Export as XSAMS

2. Levels matching

Rate coefficients

i1	F1	i2	F2	5.0	10.0	20.0	30.0	40.0	50.0
2	1	1	1	1.32E-10	1.15E-10	1.03E-10	9.76E-11	9.44E-11	9.23E-11
3	1	1	1	7.05E-11	6.26E-11	5.09E-11	4.36E-11	3.88E-11	3.55E-11
3	2	1	1	1.82E-10	1.74E-10	1.59E-10	1.5E-10	1.44E-10	1.4E-10
4	1	1	1	3.88E-11	3.63E-11	3.09E-11	2.74E-11	2.49E-11	2.32E-11
4	2	1	1	1.01E-10	1.01E-10	9.03E-11	8.13E-11	7.48E-11	7.01E-11
4	3	1	1	1.94E-10	1.81E-10	1.63E-10	1.55E-10	1.51E-10	1.49E-10
5	1	1	1	2.65E-11	2.31E-11	1.98E-11	1.8E-11	1.68E-11	1.6E-11
5	2	1	1	6.98E-11	6.84E-11	6.35E-11	5.96E-11	5.69E-11	5.49E-11
5	3	1	1	1.42E-10	1.4E-10	1.3E-10	1.21E-10	1.14E-10	1.09E-10
5	4	1	1	2.02E-10	1.97E-10	1.87E-10	1.79E-10	1.74E-10	1.71E-10
6	1	1	1	2.13E-11	2.18E-11	2.12E-11	2.04E-11	1.97E-11	1.92E-11

Einstein coefficients

upper level	lower level	frequency [MHz]	Einstein coeffic...	log(intensity)	uncertainty	upper degeneracy
2	1	87.057.535	3.89380153247...	-2.276	0.005	18
3	2	174.113.169	3.73776483149...	-1.382	0.008	30
4	3	261.164.920	0.00135166730...	-0.869	0.1	42
5	4	348.211.153	0.00332197493...	-0.516	0.04	54
6	5	435.249.668	0.00663476224...	-0.252	0.08	66
7	6	522.278.699	0.0116402293788	-0.048	0.146	78

Collider state energy and quantum numbers

state	energy[...]	degene...	parity	J	F	M	Kappa	term type	I	S	J	S2	K
1		0		0				LS	0	0			

Partition function with CDMS degeneracy

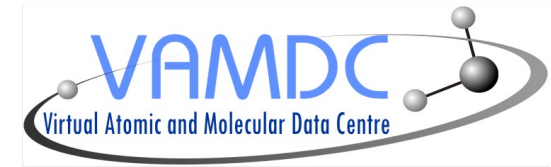
T [K]	Q
1.072	0.366
1.148	0.473
1.23	0.604
1.318	0.758
1.413	0.94
1.514	1.147
1.622	1.383
1.738	1.649
1.862	1.945
1.995	2.273
2.138	2.636

Export

* energy rate coefficients Einstein coefficients collider energy partition function save as ASCII

* save as RADEX save as XSAMS save FILE

Export data in a RADEX file



```
! Molecule
CHO+
! MASS
29.0
! Number of Energy Level
7
! LEVEL + ENERGY(CM-1) + WEIGHT + QUANTUM NOS. ElecStateLabel_J_v1_v2_v3_F_F1_F2_parity_kronigParity_r_l2_AsSym
1> 0.0> 1> X 0 0 0 0 -----
2> 2.975009> 3> X 1 0 0 0 -----
3> 8.924961> 5> X 2 0 0 0 -----
4> 17.849722> 7> X 3 0 0 0 -----
5> 29.749095> 9> X 4 0 0 0 -----
6> 44.622814> 11> X 5 0 0 0 -----
7> 62.470547> 13> X 6 0 0 0 -----
! NUMBER OF RADIATIVE TRANSITIONS
6
! TRANS + UP + LOW + EINSTEINA(s^-1) + FREQ(GHz)+ E_up(K)
1> 2> 1> 4.1868569558E-5> 8.91885247E1> 4.2805884892E0
2> 3> 2> 4.01927531801E-4> 1.783750563E2> 1.2841670504E1
3> 4> 3> 0.00145336567852> 2.675576259E2> 2.5683053237E1
4> 5> 4> 0.00357205286939> 3.56734223E2> 4.2804453237E1
5> 6> 5> 0.00713528253952> 4.459028721E2> 6.420548777E1
6> 7> 6> 0.0125158127422> 5.35061581E2> 8.9885679137E1
! NUMBER OF COLLISION PARTNERS
1
! COLLISION PARTNER
1
! COLLISIONS BETWEEN
, Scaled rate coefficients - (factor = 1.44) - Rotational collisional de-excitation rate coefficients of N2+ by He, 5K < T < 50K (Daniel & al. 2005)
! NUMBER OF COLLISIONAL TRANSITIONS
21
! NUMBER OF COLLISION TEMPERATURES
6
! COLLISION TEMPERATURES
5.0> 10.0> 20.0> 30.0> 40.0> 50.0>
! TRANS + UP + LOW + RATE COEFFS(cm^3 s^-1)
1> 2> 1> 1.9008E-10 1.656E-10 1.4832E-10 1.40544E-10 1.35936E-10 1.3291199999999997E-10
2> 3> 1> 1.0152E-10 9.0144E-11 7.3296E-11 6.2784E-11 5.5871999999999995E-11 5.112E-11
3> 3> 2> 2.6208E-10 2.5055999999999996E-10 2.2895999999999998E-10 2.1599999999999998E-10 2.0736E-10 2.016E-10
4> 4> 1> 5.5871999999999995E-11 5.2271999999999995E-11 4.449599999999999E-11 3.9455999999999997E-11 3.5856E-11 3.3408E-11
5> 4> 2> 1.4544E-10 1.4544E-10 1.30032E-10 1.17072E-10 1.07712E-10 1.0094399999999999E-10
6> 4> 3> 2.7936E-10 2.6064E-10 2.3472E-10 2.2320000000000002E-10 2.1743999999999997E-10 2.1456E-10
7> 5> 1> 3.8159999999999994E-11 3.3264E-11 2.8511999999999998E-11 2.592E-11 2.4191999999999997E-11 2.304E-11
8> 5> 2> 1.0051199999999999E-10 9.8496E-11 9.144E-11 8.5824E-11 8.1936E-11 7.9056E-11
9> 5> 3> 2.0448E-10 2.016E-10 1.8719999999999998E-10 1.7423999999999998E-10 1.6415999999999998E-10 1.5696E-10
10> 5> 4> 2.9088E-10 2.8368E-10 2.6927999999999997E-10 2.5776E-10 2.5055999999999996E-10 2.4624E-10
11> 6> 1> 3.0672E-11 3.1392E-11 3.0528E-11 2.9376E-11 2.8368E-11 2.7648E-11
12> 6> 2> 1.0296E-10 9.9936E-11 9.244799999999998E-11 8.5824E-11 8.063999999999999E-11 7.631999999999999E-11
13> 6> 3> 1.656E-10 1.6271999999999998E-10 1.4976E-10 1.38528E-10 1.29168E-10 1.21968E-10
14> 6> 4> 1.728E-10 1.7567999999999998E-10 1.6992E-10 1.6271999999999998E-10 1.5696E-10 1.512E-10
15> 6> 5> 2.0304E-10 2.016E-10 2.0304E-10 2.0448E-10 2.0592E-10 2.0879999999999997E-10
16> 7> 1> 3.2976E-11 3.2112E-11 2.9376E-11 2.6928E-11 2.4912000000000002E-11 2.3184E-11
17> 7> 2> 8.2944E-11 8.409599999999999E-11 7.891199999999999E-11 7.3296E-11 6.868799999999999E-11 6.494399999999999E-11
18> 7> 3> 1.0022399999999999E-10 1.0512000000000001E-10 1.0296E-10 9.8064E-11 9.359999999999999E-11 8.971199999999998E-11
19> 7> 4> 1.29744E-10 1.31904E-10 1.30176E-10 1.26288E-10 1.22112E-10 1.1836799999999998E-10
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