

SPECTCOL

Outil de visualisation et de traitement de données spectroscopiques et collisionnelles provenant de différentes bases de données (ex : BASECOL, CDMS, ...).

SPECTCOL Help

Import data from file

Browse... File path: collisions transitions Import

Search VAMDC databases

Databases to search: BASECOL CDMS HITRAN JPL

Species search Transitions search Collision search

Nuclear spin: Wavelength: to
Equivalent Wavelength:
Upper state energy: to
Equivalent to:
Lower state energy: to
Equivalent to:
Probability, A: to Submit query Cancel

Molecular species InChiKey:
Molecular stoichiometric formula:
Ion charge:
Atomic symbol:
Particle name:

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 stru...	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		SWQXJUGL...
2	Hyperfine collisional excitation of CN by He - 5K to 30K (Liq...	BASECOL 2...	CN	CN		JEVCWSUV...	HE	HE		SWQXJUGL...

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

Visualisation des données

Tables d'énergie

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

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

st...	en...	de...	El...	J	v1	v2	v3	F	F1	F2	pa...	kr...	r	I2	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

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 N₂ S₂H₂⁺ by He, 5K < T < 50K (Daniel & al. 2005)

Rotational collisional de-excitation rate coefficients of N₂ S₂H₂⁺ by He, 5K < T < 50K (Daniel & al. 2005)

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
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

Changer les taux de collision par un facteur

- Créer une collision $N_2H^+-H_2$ en partant de N_2H^+-He
 - Modification des Taux de Collision ($He \rightarrow H_2$)

Collisions

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

Scaled rate coef. table

Enter scaling factor:

OK Annuler

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

Scaled rate coefficients - (factor = 1.44) - Scaled rate coefficients - (factor = 1.44) - Rotational collisional de-excitation rate coefficients of N₂H⁺ + \$ by He, 5K < T < 50K (Daniel & al. 2005)

I1	F1	I2	F2	5.0	10.0	20.0	30.0	40.0	50.0
2	1	1	1	1.9008E-10	1.656E-10	1.4832E-10	1.40544E-10	1.35936E-10	1.329119999...
3	1	1	1	1.0152E-10	9.0144E-11	7.3296E-11	6.2784E-11	5.587199999...	5.112E-11
3	2	1	1	2.6208E-10	2.505599999...	2.289599999...	2.159999999...	2.0736E-10	2.016E-10
4	1	1	1	5.587199999...	5.227199999...	4.449599999...	3.945599999...	3.5856E-11	3.3408E-11
4	2	1	1	1.4544E-10	1.4544E-10	1.30032E-10	1.17072E-10	1.07712E-10	1.009439999...
4	3	1	1	2.7936E-10	2.6064E-10	2.3472E-10	2.232000000...	2.174399999...	2.1456E-10
5	1	1	1	3.815999999...	3.3264E-11	2.851199999...	2.592E-11	2.419199999...	2.304E-11
5	2	1	1	1.005119999...	9.8496E-11	9.144E-11	8.5824E-11	8.1936E-11	7.9056E-11
5	3	1	1	2.0448E-10	2.016E-10	1.871999999...	1.742399999...	1.641599999...	1.5696E-10
5	4	1	1	2.9088E-10	2.8368E-10	2.692799999...	2.5776E-10	2.505599999...	2.4624E-10
6	1	1	1	3.0672E-11	3.1392E-11	3.0528E-11	2.9376E-11	2.8368E-11	2.7648E-11
6	2	1	1	1.0296E-10	9.936E-11	9.244799999...	8.5824E-11	8.063999999...	7.631999999...
6	3	1	1	1.656E-10	1.627199999...	1.4976E-10	1.38528E-10	1.29168E-10	1.21968E-10
6	4	1	1	1.728E-10	1.756799999...	1.6992E-10	1.627199999...	1.5696E-10	1.512E-10
6	5	1	1	2.0304E-10	2.016E-10	2.0304E-10	2.0448E-10	2.0592E-10	2.087999999...
7	1	1	1	3.2976E-11	3.2112E-11	2.9376E-11	2.6928E-11	2.491200000...	2.3184E-11
7	2	1	1	8.2944E-11	8.409599999...	7.891199999...	7.3296E-11	6.868799999...	6.494399999...
7	3	1	1	1.002239999...	1.051200000...	1.0296E-10	9.8064E-11	9.359999999...	8.971199999...
7	4	1	1	1.29744E-10	1.31904E-10	1.30176E-10	1.26288E-10	1.22112E-10	1.183679999...
7	5	1	1	1.4976E-10	1.526399999...	1.5408E-10	1.512E-10	1.4832E-10	1.4544E-10
7	6	1	1	1.7856E-10	1.771199999...	1.771199999...	1.7856E-10	1.8288E-10	1.8576E-10

save as ASCII

Collisions

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

Scaled collisions

	comment	source	target stru...	target stoi...	target spin	target InCh...	collider stru...	collider stoi...	collider spin	collider InC...
1	f=1... Scaled rate coefficients - (factor = 1.44) - Rotational collisional de-excitation rate coefficients of N ₂ H ⁺ + \$ by He, 5K < T < 50K (Daniel & al. 2005)	BASECOL 2...	\$N_2H^+ + \$	HN2+		GRMHOSH...	HE	HE		SWQXJQGL...

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

Association de données spectroscopiques et collisionnelles(2/2)

Selection spectro et collision

Résultat : combinaison spectro et collision

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- v 1:HC...	CDMS 2014-07-...	HCO-17+	CHO+		XPRMKTHGXOVK...
4	31506- v 1: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- v 1:DO...	CDMS 2014-07-...	DOC+	CHO+		FIRPXVMTWVP...
11	29505- v 1: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	Hyperf...	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

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 coeffie...	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	261,164.92	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	l	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 RADEX save as XSAMS

Sortie RADEX

```
! 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 N$2$H$^+$ 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 2.5059999999999996E-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 1.009439999999999E-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 9.2447999999999998E-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 8.971199999999999E-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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